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**Effective Discontinuous Interface Coupled Models  
for Atomistic Energy Minimisation**

By

*Eleftheria Karnesis*

A thesis submitted in partial fulfillment for the  
degree of Doctor of Philosophy

in the  
School of Mathematical and Physical Sciences  
University of Sussex

June 2019

# Declaration

I hereby declare that this thesis has not been and will not be, submitted in whole or in part to another University for the award of any other degree.

Signature .....

Eleftheria Karnesis

# Dedication

To my parents, sister and brother;  
Spyros, Vassiliki, Angelique and Nicholas

μηδενὶ μηδὲν ὀφείλετε εἰ μὴ τὸ ἀγαπᾶν ἀλλήλους.

Saint Paul

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UNIVERSITY OF SUSSEX

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SUBMITTED FOR THE DEGREE OF DOCTOR OF  
PHILOSOPHY

EFFECTIVE DISCONTINUOUS INTERFACE COUPLED MODELS FOR  
ATOMISTIC ENERGY MINIMISATION

### SUMMARY

In the field of multiscale modelling of materials, a class of significant problems involves the atomistic-to-continuum coupling in crystals. Continuum models frequently fail to produce accurate predictions near singularities and defects and hence coupled atomistic/continuum methods have become popular. The ad-hoc coupling of atomistic and continuum energies results in numerical artifacts on the interface between the continuum and atomistic regions, known as ghost forces. The design and analysis of atomistic/continuum coupling methods that are ghost-force free is important in computational and mathematical modelling of materials and one of the very few well defined problems in multi-scale algorithm design for nonlinear phenomena.

In this thesis we developed a discontinuous ghost-force free bond volume based method in one dimensional and two dimensional crystal lattices. The design of the method was motivated by appropriately analysing the error both at the atomistic and the continuum region. Its design is consistent and transferable. Next, we were concerned about the energy consistency and the variational consistency of the coupled methods. Consistency is a quantity that measures the extent to which an exact smooth solution does satisfy the numerical scheme. We proved that in one dimension the local contributions of the energy were of second order in the lattice spacing  $\varepsilon$ ,  $O(\varepsilon^2)$ . The total energy error in one and two dimensions was second order. We analysed the error for first variations both in one and two dimensions. Our analysis confirmed that the proposed methods were indeed ghost-force free and their variational consistency error was bounded by  $(\varepsilon^2 + \varepsilon^{2-\frac{1}{p}})$  in the discrete  $W^{-1,p}$  norm. We implemented the static atomistic problem and compared it to the static coupled method in one dimension. We considered energies from multi-body potentials. By using the symmetry properties of the potentials we derived energy consistency error bounds of order  $O(\varepsilon^2)$ .

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# Chapter 1

## Introduction

The accurate theoretical prediction of the mechanical properties, and specifically the mechanical responses, of crystalline materials under internal and/or external loads, require analytical approaches which take into account the atomic structure of the material and the atomic interconnection/interrelation between microcrystals. At a higher characteristic length-level the atom, treated as an entity, is considered the sole factor determining the behavior of the material. At this level, a number of models such as Lennard-Jones and Morse, attempting to describe the interatomic potential energy in classical terms, were developed over the years. These models may describe with certain level of accuracy the mechanical behaviour of specific kinds of crystals. However, simulating such atomistic systems is very demanding from a computational perspective mainly due to the number of the degrees of freedom (say one per atom) which is prohibitively large, even for nanostructures. On the other hand, the computational cost cannot always be reduced by considering effective continuum models, since such models are available only in restrictive situations, excluding interesting phenomena, such as defects, cracks etc. From a methodological perspective these problems are related to several other challenges in prediction of singular phenomena. For example, interfaces and defects play an important role in nanomechanics as they relate to nanostructures [16] and fracture and crack propagation models are becoming very important in other areas as well, e.g. in seismology [34].

To address this challenge several attempts have been made over the years. Most of them were based on the combination of models across scales, termed *multiscale models*. Substantial progress has been made in recent years, in the field of multiscale modeling of materials, see e.g., [5, 17].

A multiscale approach that has received considerable attention from the engineering as well as from the mathematical point of view, is the atomistic-to-continuum passage [9, 4, 2, 8, 21, 27], and the corresponding atomistic-to-continuum coupled methods for crystalline materials, e.g., [31, 3, 5, 7, 23, 20]. These methods relate to the quasicontinuum method [31] and its variants. Close to defects and singularities, continuum models fail to produce accurate results and so coupled atomistic/continuum (A/C) methods are being used as an adaptive approach; see, for example, the references in [21, 1, 29, 15, 22, 32, 33, 30, 24, 25, 18].

This thesis concerns the analysis and the design of new atomistic/continuum coupled methods in crystalline structures. These methods can be seen as variants of the “quasicontinuum” method [31]. In these methods, in regions of interest in the

material (interfaces, defects, localized deformations) the atomistic model is kept, while in regions of smooth deformations it is replaced with a continuum model discretized by finite elements. Despite the increasing number of papers concerned with the numerical analysis of these methods, satisfactory analytical results are available in limited cases only. This thesis introduces and analyses a flexible and systematic class of methods based on adding discontinuous interface terms providing the right correction and exchange of information mechanisms between atomistic and continuum regions. Our analysis can be extended by similar and tedious calculations in three dimensions.

## 1.1 Definitions and Notation

Let  $\mathcal{L}_{entire} = \mathbb{Z}^2$  be a two-dimensional lattice that is generated from two linearly independent vectors  $e_1, e_2$  of  $\mathbb{R}^2$ . Consider discrete periodic functions of  $\mathcal{L}_{entire}$  defined over a ‘periodic domain’  $\mathcal{L}$ . Let

$$\mathcal{L} = \{\ell = (\ell_1, \ell_2) \in [1, N] \times [1, N], \quad N \in \mathbb{N}\}.$$

Let  $\varepsilon$  be the interatomic spacing. The configuration of the atoms before deformation is defined as

$$\Omega_{discr} = \{x_\ell = (x_{\ell_1}, x_{\ell_2}) = (\varepsilon\ell_1, \varepsilon\ell_2), \quad \ell_1 \in [1, N], \quad \ell_2 \in [1, N]\},$$

$$\Omega = \{x \in [x_1, x_{N+1}] \times [x_1, x_{N+1}]\}.$$

Let  $y : [1, N] \times [1, N] \rightarrow \mathbb{R}^2$  be the atomistic deformation such that, for  $\ell \in \mathcal{L}$ ,

$$y_\ell = y(x_\ell) = y(x_{\ell_1}, x_{\ell_2}) = \begin{bmatrix} y^1(x_{\ell_1}, x_{\ell_2}) \\ y^2(x_{\ell_1}, x_{\ell_2}) \end{bmatrix}. \quad (1.1)$$

Specifically, the affine atomistic deformation is

$$\begin{bmatrix} y^1(x_{\ell_1}, x_{\ell_2}) \\ y^2(x_{\ell_1}, x_{\ell_2}) \end{bmatrix} = \begin{bmatrix} F_{11} & F_{12} \\ F_{21} & F_{22} \end{bmatrix} \begin{bmatrix} x_{\ell_1} \\ x_{\ell_2} \end{bmatrix} + \begin{bmatrix} v^1(x_{\ell_1}, x_{\ell_2}) \\ v^2(x_{\ell_1}, x_{\ell_2}) \end{bmatrix} \quad (1.2)$$

or  $y_\ell = Fx_\ell + v_\ell$ , where  $v_\ell = v(x_{\ell_1}, x_{\ell_2})$  is periodic with respect to  $\mathcal{L}$  and  $F$  is a constant  $2 \times 2$  deformation gradient matrix with  $\det(F) > 0$ .

The function spaces for  $y$  and  $v$  are denoted by  $\mathcal{X}$  and  $\mathcal{V}$ , respectively and are defined as, [21]

$$\begin{aligned} \mathcal{X} &:= \{y : \mathcal{L} \rightarrow \mathbb{R}^2, \quad y_\ell = Fx_\ell + v_\ell, \quad v \in \mathcal{V}, \quad \ell \in \mathcal{L}\}, \\ \mathcal{V} &:= \{u : \mathcal{L} \rightarrow \mathbb{R}^2, \quad u_\ell = u(x_\ell) \quad \text{periodic with zero average with respect to } \mathcal{L}\}. \end{aligned}$$

For functions  $y, v : \mathcal{L} \rightarrow \mathbb{R}^2$  we define the inner product

$$\langle y, v \rangle_\varepsilon := \varepsilon^2 \sum_{\ell \in \mathcal{L}} y_\ell \cdot v_\ell.$$

For  $1 \leq p \leq \infty$  and a positive real number  $s$  the Sobolev space for functions  $y : \Omega \rightarrow \mathbb{R}^2$  is denoted by  $W^{s,p}(\Omega, \mathbb{R}^2)$ . The corresponding Sobolev space of functions that are periodic with basic period  $\Omega$  is denoted by  $W_{\#}^{s,p}(\Omega, \mathbb{R}^2)$ . By  $\langle \cdot, \cdot \rangle$  we denote the standard  $L^2(\Omega)$  inner product; for a given nonlinear operator  $A$ , we shall denote

as well by  $\langle DA, v \rangle$  the action of its derivative  $DA$  as a linear operator applied to  $v$ . The continuum space corresponding to the function space  $\mathcal{X}$  is, [21]

$$\begin{aligned} X &:= \{y : \Omega \rightarrow \mathbb{R}^2, \quad y(x) = Fx + v(x), \quad v \in V\}, \quad \text{where} \\ V &:= \{u : \Omega \rightarrow \mathbb{R}^2, \quad u \in W^{k,p}(\Omega, \mathbb{R}^2) \cap W_{\#}^{1,p}(\Omega, \mathbb{R}^2), \quad \int_{\Omega} u dx = 0\}. \end{aligned}$$

We will further use the notation

$$\nabla_{\zeta} \phi(\zeta) := \begin{bmatrix} \frac{\partial \phi(\zeta)}{\partial \zeta_1} \\ \frac{\partial \phi(\zeta)}{\partial \zeta_2} \end{bmatrix} \quad (1.3)$$

and

$$\nabla u(x) := \begin{bmatrix} \frac{\partial u^1(x)}{\partial x_1} & \frac{\partial u^1(x)}{\partial x_2} \\ \frac{\partial u^2(x)}{\partial x_1} & \frac{\partial u^2(x)}{\partial x_2} \end{bmatrix}. \quad (1.4)$$

## 1.2 Atomistic and Cauchy–Born potential

Let  $R$  be a finite set of given interaction vectors, as follows

$$R = \{\eta = (\eta_1, \eta_2) \in [-N_{R_1}, N_{R_1}] \times [-N_{R_2}, N_{R_2}], \quad N_{R_1}, N_{R_2} \in \mathbb{N}\}, \quad (1.5)$$

where  $N_{R_1} \ll N$  and  $N_{R_2} \ll N$ . Then for  $\eta \in R$  and  $\ell \in \mathcal{L}$ , the difference quotient is defined as

$$\overline{D}_{\eta} y_{\ell} = \frac{y_{\ell+\eta} - y_{\ell}}{\varepsilon} = \begin{bmatrix} \frac{y^1(x_{\ell_1+\eta_1}, x_{\ell_2+\eta_2}) - y^1(x_{\ell_1}, x_{\ell_2})}{\varepsilon} \\ \frac{y^2(x_{\ell_1+\eta_1}, x_{\ell_2+\eta_2}) - y^2(x_{\ell_1}, x_{\ell_2})}{\varepsilon} \end{bmatrix}. \quad (1.6)$$

Consider the following atomistic potential

$$\Phi^a(y) := \varepsilon^2 \sum_{\ell \in \mathcal{L}} \sum_{\eta \in R} \phi(\overline{D}_{\eta} y_{\ell}). \quad (1.7)$$

We will make some assumptions for the atomistic potential:

**Assumption 1.** *The functions  $\phi(\zeta)$  are defined on  $\mathbb{R}^2 \setminus \{0\}$ , [4] and they are smooth for any  $\zeta$ ,  $|\zeta| > \rho$ .*

**Assumption 2.** *There exists a  $C_{\rho,k} = C(\rho, k) \geq 0$ , such that for  $|\zeta| > \rho$ ,  $|D_{\zeta}^k \phi(\zeta)| \leq C_{\rho,k}$ , and  $k$  is a multi-index with  $|k| \leq 2$ .*

Notice that we do not need symmetry assumptions on the potentials  $\phi$  with the exception of the multi-body potentials considered at the last chapter of the thesis. Sufficiently smooth diffeomorphisms  $y$  on the domain  $\Omega$  will be considered for the analysis of the consistency of the Cauchy–Born approximation.

**Assumption 3.** *In order to exclude interpenetration we need to assume that  $y$  is  $1 - 1$ . Furthermore, it leads to the following lower bound  $|\overline{D}_\eta y_\ell| \geq \alpha(y, \eta) > 0$ , [4], needed to bound derivatives of  $\phi(\overline{D}_\eta y_\ell)$ .*

The atomistic problem is:

$$\begin{aligned} &\text{find } y^a, \text{ a local minimizer in } \mathcal{X} \text{ of :} \\ &\Phi^a(y) - \langle f, y \rangle_\varepsilon \end{aligned} \quad (1.8)$$

where  $f : \mathcal{L} \rightarrow \mathbb{R}^2$ ,  $f_\ell = f(x_\ell)$ , is a given field of external forces. If this minimizer exists, then for all  $v \in \mathcal{V}$

$$\langle D\Phi^a(y^a), v \rangle_\varepsilon = \langle f, v \rangle_\varepsilon, \quad (1.9)$$

where

$$\begin{aligned} \langle D\Phi^a(y), v \rangle_\varepsilon &= \varepsilon^2 \sum_{\ell \in \mathcal{L}} \sum_{\eta \in R} \partial_{\zeta_i} \phi_\eta(\overline{D}_\eta y_\ell) [\overline{D}_\eta v_\ell]_i \\ &= \varepsilon^2 \sum_{\ell \in \mathcal{L}} \sum_{\eta \in R} \nabla_\zeta \phi_\eta(\overline{D}_\eta y_\ell) \cdot \overline{D}_\eta v_\ell. \end{aligned} \quad (1.10)$$

Here and throughout we use the Einstein summation convention for repeated indices. The Cauchy–Born stored energy function is

$$W(F) = W_{CB}(F) = \sum_{\eta \in R} \phi_\eta(F\eta) \quad (1.11)$$

and, the continuum Cauchy–Born model is:

$$\begin{aligned} &\text{find } y^{CB}, \text{ a local minimizer in } X \text{ of :} \\ &\Phi^{CB}(y) - \langle f, y \rangle, \end{aligned} \quad (1.12)$$

where

$$\Phi^{CB}(y) := \int_{\Omega} W_{CB}(\nabla y(x)) dx \quad (1.13)$$

and  $f$ , the external forces, are related appropriately to the discrete external forces. If this minimizer exists, then for all  $v \in V$ ,

$$\langle D\Phi^{CB}(y^{CB}), v \rangle = \langle f, v \rangle, \quad (1.14)$$

where

$$\langle D\Phi^{CB}(y), v \rangle = \int_{\Omega} S_{i\alpha}(\nabla y(x)) \frac{\partial v^i(x)}{\partial x_\alpha} dx = \int_{\Omega} S_{i\alpha}(\nabla y(x)) \partial_\alpha v^i(x) dx, \quad v \in V. \quad (1.15)$$

The stress tensor  $S$  is

$$S := \left\{ \frac{\partial W(F)}{\partial F_{i\alpha}} \right\}_{i\alpha}. \quad (1.16)$$

The relation between the atomistic potential and the stress tensor is:

$$\begin{aligned}
 S_{i\alpha} &= \frac{\partial W(\mathbf{F})}{\partial F_{i\alpha}} = \frac{\partial}{\partial F_{i\alpha}} \sum_{\eta \in R} \phi_{\eta}(\mathbf{F} \eta) \\
 &= \frac{\partial}{\partial F_{i\alpha}} \sum_{\eta \in R} \phi_{\eta}(F_{j\beta} \eta_{\beta}) = \sum_{\eta \in R} \partial_{\zeta_i} \phi_{\eta}(F_{j\beta} \eta_{\beta}) \frac{\partial}{\partial F_{i\alpha}} F_{j\beta} \eta_{\beta} \\
 &= \sum_{\eta \in R} \partial_{\zeta_i} \phi_{\eta}(\mathbf{F} \eta) \eta_{\alpha}.
 \end{aligned} \tag{1.17}$$

### 1.2.1 Crystalline Structures and Potential energy functions

Most solids have a crystalline structure, which means that the atoms have a periodic pattern arrangement. The study of solids has been boosted significantly by the existence of crystals because in order to analyse a crystalline solid it is necessary to consider what happens in a unit of the crystal, or a unit cell. This unit cell is then repeated periodically in the three dimensions to form the perfect and infinite solid. At the quantum scale, the origin of the properties of solids is the interaction between the valence electrons, i.e. the electrons that are on the outershells of atoms. The valence electrons interact between each other, and with the constituent atom's nuclei. At the atomistic scale considered herein, each atom is treated as an entity, and the properties of the solid are determined by the atomic structure.

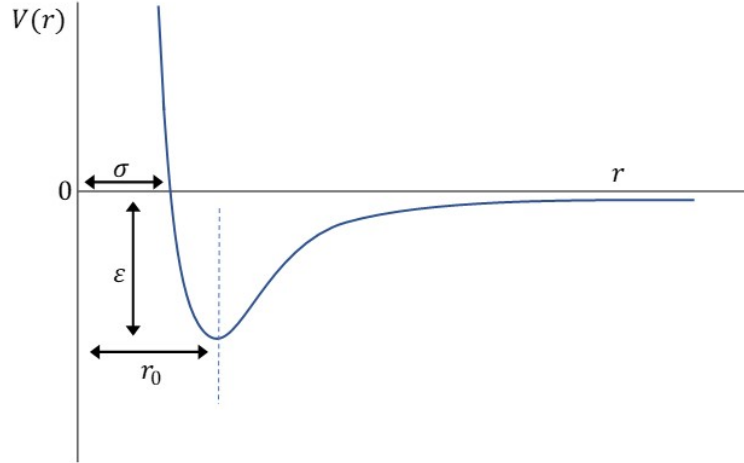
Interatomic potentials are functions which are used to calculate the potential energy of a whole system of atoms where the atoms are in given positions in space. The most important interatomic potentials are the pair potentials, which is the potential of the interaction of two atoms, and the many-body potentials. In this thesis we will use pair potentials in the analysis except in Chapter 6 where the theory is for many-body potentials. The interatomic pair potential is obtained by adding the repulsive and attractive potentials, [10]. When two atoms are very close together they have a repulsive force between each other and when two atoms are apart from each other they have an attractive force between them which decreases the further apart they are. The most known pair potential is the Lennard-Jones, or "6-12" potential

$$\phi(r) = 4\epsilon \left[ \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^6 \right], \tag{1.18}$$

where  $r$  is the distance between the two atoms,  $\epsilon$  is the bond energy at the equilibrium position  $r_0$  and  $\sigma$  is the interatomic distance when the potential is zero, Figure 1.1. Thus,  $\phi(r) = 0$  when  $r = \sigma$  and when  $r = 2^{\frac{1}{6}}\sigma$ , the minimum energy occurs. Another interatomic pair potential is the Morse potential

$$V(r) = D_e(1 - e^{-a(r-r_e)})^2, \tag{1.19}$$

where  $D_e$  is the well depth,  $r$  is the interatomic distance,  $r_e$  is the distance between the atoms where the potential energy is at a minimum and  $a$  is a parameter that controls the width of the potential. Both of these potentials satisfy the assumptions in Section 1.2. They will be used in the numerical simulations in the end of Chapter 3, Section 3.4.



**Figure 1.1:** The Lennard-Jones potential.

### 1.2.2 Atomistic Cauchy–Born model

We link the atomistic model and the continuous model with an intermediate model, the *atomistic Cauchy–Born model (A-CB)*, [21]. Throughout the thesis, this model is used as an analytical tool in order to design the coupled methods. An important feature of the A-CB model is the fact that its consistency error is  $\mathcal{O}(\varepsilon^2)$  when compared to the continuous Cauchy–Born model for both the energy and the first variations.

Let  $\mathbb{V}_{\varepsilon,Q}(Q)$  be defined as the space of piecewise continuous bilinear periodic functions on  $\mathcal{L}$ , the lattice. Let

$$\begin{aligned} \mathcal{T}_Q &:= \{K \subset \Omega : K = K_\ell = (x_{\ell_1}, x_{\ell_1+1}) \times (x_{\ell_2}, x_{\ell_2+1}), \quad x_\ell = (x_{\ell_1}, x_{\ell_2}) \in \Omega_{\text{discr}}\}, \\ \mathbb{V}_{\varepsilon,Q} &:= \{v : \bar{\Omega} \rightarrow \mathbb{R}^2, \quad v \in C(\bar{\Omega}), \quad v|_K \in \mathbb{Q}_1(K) \text{ and} \\ &\quad v_\ell = v(x_\ell) \text{ is periodic with respect to } \mathcal{L}\}, \end{aligned} \tag{1.20}$$

where the set of bilinear functions on  $K$  is denoted by  $\mathbb{Q}_1(K)$ , [21]. The space  $\mathbb{V}_{\varepsilon,Q}$  is the standard finite element space consisting of bilinear elements. For any connected set  $\mathcal{O}$  that satisfies  $\bar{\mathcal{O}} = \overline{\cup_{K \in \mathcal{S}_Q} K}$ , where  $\mathcal{S}_Q$  is a subset of  $\mathcal{T}_Q$  we let  $\mathbb{V}_{\varepsilon,Q}(\mathcal{O})$  denote the natural restriction of  $\mathbb{V}_{\varepsilon,Q}$  on the set  $\mathcal{O}$ . This space will be instrumental for the thesis. In particular, it provides a link between discrete atomistic values and functions, defined in the entire domain, and thus will help us to compare discrete and continuum functions.

The average discrete derivatives are defined as follows:

$$\begin{aligned} \bar{\bar{D}}_{e_1} v_\ell &:= \frac{1}{2} \left\{ \bar{D}_{e_1} v_\ell + \bar{D}_{e_1} v_{\ell+e_2} \right\}, \\ \bar{\bar{D}}_{e_2} v_\ell &:= \frac{1}{2} \left\{ \bar{D}_{e_2} v_\ell + \bar{D}_{e_2} v_{\ell+e_1} \right\}. \end{aligned} \tag{1.21}$$

The discrete gradient matrix can be defined as

$$\left\{ \bar{\nabla} v_\ell \right\}_{i\alpha} = \bar{\bar{D}}_{e_\alpha} v_\ell^i. \tag{1.22}$$



Here, the atomistic Cauchy–Born potential is

$$\begin{aligned}\Phi^{a,CB}(y) &= \varepsilon^d \sum_{\ell \in \mathcal{L}} \sum_{\eta \in R} \phi_\eta(\bar{\nabla} y_\ell \eta) \\ &= \varepsilon^d \sum_{\ell \in \mathcal{L}} W_{CB}(\bar{\nabla} y_\ell).\end{aligned}\tag{1.23}$$

The *atomistic Cauchy–Born* problem is:

$$\begin{aligned}\text{find } y^{a,CB}, \text{ a local minimizer in } \mathcal{X} \text{ of :} \\ \Phi^{a,CB}(y) - \langle f, y \rangle_\varepsilon,\end{aligned}\tag{1.24}$$

where  $f : \mathcal{L} \rightarrow \mathbb{R}^d$  are a given field of external forces. If this minimizer exists, then for all  $v \in \mathcal{V}$

$$\langle D\Phi^{a,CB}(y^{a,CB}), v \rangle_\varepsilon = \langle f, v \rangle_\varepsilon.\tag{1.25}$$

The quality of the approximation of the CB-model becomes evident by comparing  $W_{CB}(\bar{\nabla} y_\ell)$  to  $W_{CB}(\nabla y(m_K))$ , where  $y$  is a smooth function, and  $m_K$  is the bary-center of  $K$ , where  $K$  is the element with vertices  $x_\ell$ ,  $x_{\ell+e_1}$ ,  $x_{\ell+e_1+e_2}$ ,  $x_{\ell+e_2}$ , and  $y(x_\ell) = y_\ell$ . A key property is that

$$\nabla y(m_K) = \bar{\nabla} y_\ell, \quad \text{for } y \in \mathbb{V}_{\varepsilon,Q}.\tag{1.26}$$

Then, cf. [21], for any  $v \in \mathbb{V}_{\varepsilon,Q}$ , the quantity

$$\begin{aligned}\langle \mathcal{A}^{a,CB}, v \rangle_\varepsilon &:= \varepsilon^d \sum_{K \in \mathcal{T}} \sum_{\eta \in R} \{S_{i1}(\nabla y(m_K))\} \left[ \frac{1}{2} \left\{ \bar{D}_{e_1} v_\ell + \bar{D}_{e_1} v_{\ell+e_2} \right\} \right]_i \\ &\quad + \varepsilon^d \sum_{K \in \mathcal{T}} \sum_{\eta \in R} \{S_{i2}(\nabla y(m_K))\} \left[ \frac{1}{2} \left\{ \bar{D}_{e_2} v_\ell + \bar{D}_{e_2} v_{\ell+e_1} \right\} \right]_i \\ &= \varepsilon^d \sum_{K \in \mathcal{T}} \sum_{\eta \in R} \{ \nabla_\zeta \phi_\eta(\nabla y(m_K) \eta) \eta_1 \} \frac{1}{2} \left\{ \bar{D}_{e_1} v_\ell + \bar{D}_{e_1} v_{\ell+e_2} \right\} \\ &\quad + \varepsilon^d \sum_{K \in \mathcal{T}} \sum_{\eta \in R} \{ \nabla_\zeta \phi_\eta(\nabla y(m_K) \eta) \eta_2 \} \frac{1}{2} \left\{ \bar{D}_{e_2} v_\ell + \bar{D}_{e_2} v_{\ell+e_1} \right\},\end{aligned}\tag{1.27}$$

is an approximation of second order to the quantity  $\langle D\Phi^{CB}(y), v \rangle$ . This means that a constant  $M = M(y, p)$ ,  $1 \leq p \leq \infty$ , exists, which is independent of  $v$ , such that

$$\left| \langle D\Phi^{CB}(y), v \rangle - \langle \mathcal{A}^{a,CB}, v \rangle_\varepsilon \right| \leq M \varepsilon^2 |v|_{W^{1,p}(\Omega)}.\tag{1.28}$$

The next lemma provides a link between  $\mathcal{A}^{a,CB}$  and  $D\Phi^{a,CB}$  [21].

**Lemma 1.** *Let  $y \in \mathbb{V}_{\varepsilon,Q}$ ; then*

$$\langle \mathcal{A}^{a,CB}, v \rangle_\varepsilon = \langle D\Phi^{a,CB}(y), v \rangle_\varepsilon, \text{ for any } v \in \mathbb{V}_{\varepsilon,Q}.\tag{1.29}$$

*Proof.* Firstly,

$$\begin{aligned}\langle D\Phi^{a,CB}(y), v \rangle_\varepsilon &= \varepsilon^d \sum_{\ell \in \mathcal{L}} \sum_{\eta \in R} \{S_{i1}(\bar{\nabla} y_\ell)\} \left[ \frac{1}{2} \left\{ \bar{D}_{e_1} v_\ell + \bar{D}_{e_1} v_{\ell+e_2} \right\} \right]_i \\ &\quad + \varepsilon^d \sum_{\ell \in \mathcal{L}} \sum_{\eta \in R} \{S_{i2}(\bar{\nabla} y_\ell)\} \left[ \frac{1}{2} \left\{ \bar{D}_{e_2} v_\ell + \bar{D}_{e_2} v_{\ell+e_1} \right\} \right]_i.\end{aligned}\tag{1.30}$$

Therefore, since  $y \in \mathbb{V}_{\varepsilon, Q}$  (1.26), then  $S_{i\alpha}(\nabla y(m_K)) = S_{i\alpha}(\bar{\nabla} y_\ell)$ .  $\square$

The atomistic CB model is *consistent*, meaning that *homogeneous* deformations,  $y_F(x) = Fx$ ,  $x \in \Omega$ , are its critical points. A property which it shares with both the continuum and the atomistic models. We have

$$\langle D\Phi^{a,CB}(y_F), v \rangle = 0, \quad y_F(x) = Fx, \quad (1.31)$$

for all  $v \in \mathbb{V}_{\varepsilon, Q}$ . This is implied by

$$\begin{aligned} \langle D\Phi^{a,CB}(y_F), v \rangle &= \varepsilon^2 \sum_{\ell \in \mathcal{L}} \sum_{\eta \in R} \nabla_\zeta \phi_\eta(\bar{\nabla} y_F \eta) \cdot \bar{\nabla} v \eta \\ &= \sum_{\eta \in R} \nabla_\zeta \phi(F \eta) \cdot \sum_{\ell \in \mathcal{L}} \varepsilon^3 \bar{\nabla} v \eta \\ &= \sum_{\eta \in R} \nabla_\zeta \phi(F \eta) \cdot \sum_{\ell \in \mathcal{L}} \int_{K_\ell} \nabla v \eta \, dx \\ &= \sum_{\eta \in R} \nabla_\zeta \phi(F \eta) \cdot \int_{\Omega} \nabla v \eta \, dx = 0, \end{aligned} \quad (1.32)$$

where the last integral is zero due to periodicity. In [21] it was shown that this model is energy- as well as variationally consistent to second order in interatomic spacing  $\varepsilon$ , approximating both the continuum Cauchy-Born model and the exact atomistic model.

## 1.3 Design principles of the coupling methods

We define  $\Omega_a$  as the atomistic region,  $\Omega_*$  as the atomistic Cauchy-Born region and  $\Gamma$  as the interface between  $\Omega_a$  and  $\Omega_*$  which has no thickness. Also,  $\Omega$  is the whole region being examined which contains  $\Omega_a$ ,  $\Omega_*$  and  $\Gamma$  such that

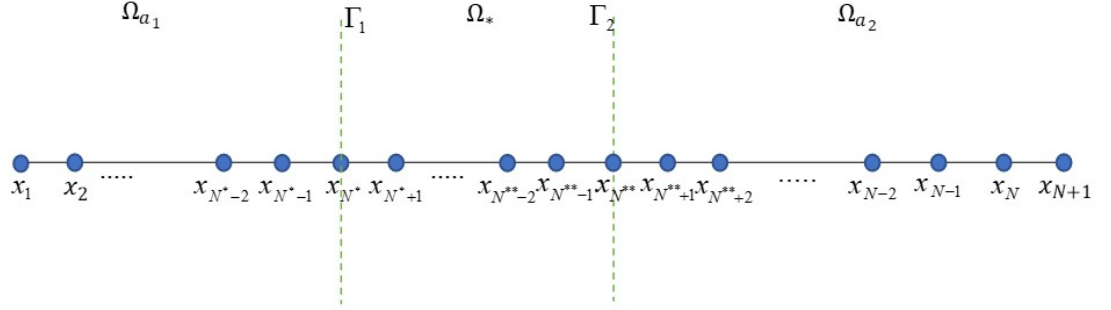
$$\bar{\Omega} = \bar{\Omega}_a \cup \bar{\Omega}_*, \quad \Gamma = \bar{\Omega}_a \cap \bar{\Omega}_*.$$

Notice that at a first stage it is convenient to use as "continuum region" the atomistic Cauchy-Born region for technical reasons. The continuum Cauchy-Born model discretised by finite elements of arbitrary degree can be used in  $\Omega_*$ , subsequently, see [19] for details. In one dimension we have two atomistic regions  $\Omega_{a_1}$  and  $\Omega_{a_2}$  and the atomistic Cauchy-Born region is  $\Omega_*$  which are on a line and the  $\Gamma_1$  and  $\Gamma_2$  interfaces are two points as displayed in Figure 1.2. In two dimensions the atomistic region is split into four sections  $\Omega_{a_1}$ ,  $\Omega_{a_2}$ ,  $\Omega_{a_3}$  and  $\Omega_{a_4}$  for convenience. The atomistic Cauchy-Born region is  $\Omega_*$  and the interface is split into four sections  $\Gamma_1$ ,  $\Gamma_2$ ,  $\Gamma_3$  and  $\Gamma_4$  as displayed in Figure 1.3.

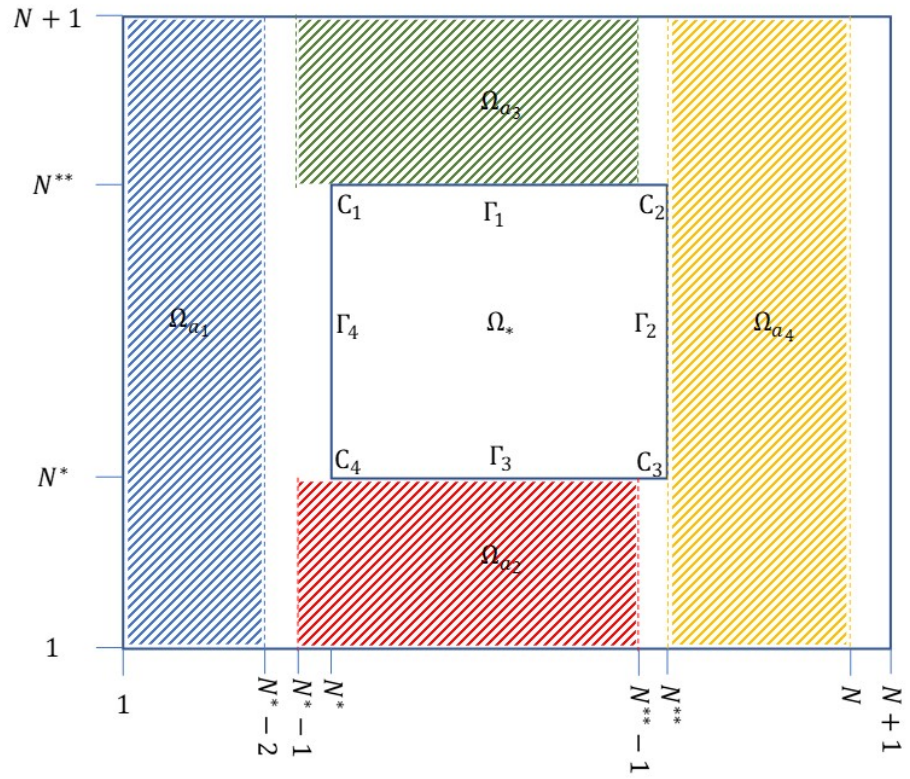
For a fixed  $\eta \in R$  a bond can be defined as the line segment  $b_\ell = \{x \in \mathbb{R}^2: x = \ell + t\eta, 0 < t < 1\}$ . A *bond volume*  $B_{\ell, \eta}$  that corresponds to  $b_\ell$  is the interior part of a parallelogram that has a diagonal  $b_\ell$ , i.e.,

$$B_{\ell, \eta} \text{ is an open quadrilateral that has vertices } x_\ell, x_{\ell+\eta_1 e_1}, x_{\ell+\eta_2 e_2}, x_{\ell+\eta}. \quad (1.33)$$

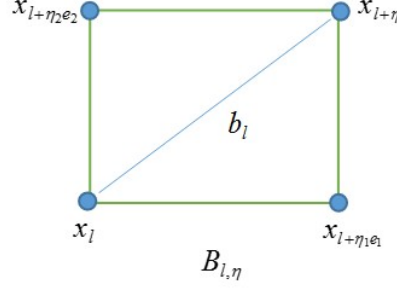
which is displayed in Figure 1.4. The following lemma will be useful in this thesis.



**Figure 1.2:** The regions  $\Omega_a$  and  $\Omega_*$  and the interfaces  $\Gamma_1$  and  $\Gamma_2$ .



**Figure 1.3:** Displaying  $\Omega_{a_1}, \Omega_{a_2}, \Omega_{a_3}, \Omega_{a_4}, \Omega_*$  and the interfaces  $\Gamma_1, \Gamma_2, \Gamma_3, \Gamma_4$

Figure 1.4: The bond volume  $B_{\ell, \eta}$ 

**Lemma 2.** Let  $v \in \mathbb{Q}_1(B_{\ell, \eta})$ . Then

$$\varepsilon^2 \overline{D}_\eta v_\ell = \frac{1}{\eta_1 \eta_2} \int_{B_{\ell, \eta}} \nabla v(x) \cdot \eta \, dx. \quad (1.34)$$

*Proof.* Firstly,

$$\begin{aligned} \frac{1}{\eta_1 \eta_2} \int_{B_{\ell, \eta}} \nabla v(x) \cdot \eta \, dx &= \frac{1}{\eta_1 \eta_2} \int_{\partial B_{\ell, \eta}} \nu \cdot \eta v \, ds \\ &= \frac{1}{\eta_1 \eta_2} \left\{ \int_{(x_\ell, x_{\ell+\eta_1 e_1})} (-\eta_2) v \, ds + \int_{(x_{\ell+\eta_2 e_2}, x_{\ell+\eta})} \eta_2 v \, ds \right. \\ &\quad \left. + \int_{(x_\ell, x_{\ell+\eta_2 e_2})} (-\eta_1) v \, ds + \int_{(x_{\ell+\eta_1 e_1}, x_{\ell+\eta})} \eta_1 v \, ds \right\}. \end{aligned} \quad (1.35)$$

At each edge of  $B_{\ell, \eta}$ ,  $v$  is linear, and therefore

$$\int_{(x_\ell, x_{\ell+\eta_1 e_1})} (-\eta_2) v \, ds + \int_{(x_{\ell+\eta_2 e_2}, x_{\ell+\eta})} \eta_2 v \, ds = \frac{\varepsilon \eta_1 \eta_2}{2} (v_{\ell+\eta} + v_{\ell+\eta_2 e_2} - v_{\ell+\eta_1 e_1} - v_\ell). \quad (1.36)$$

We finally obtain,

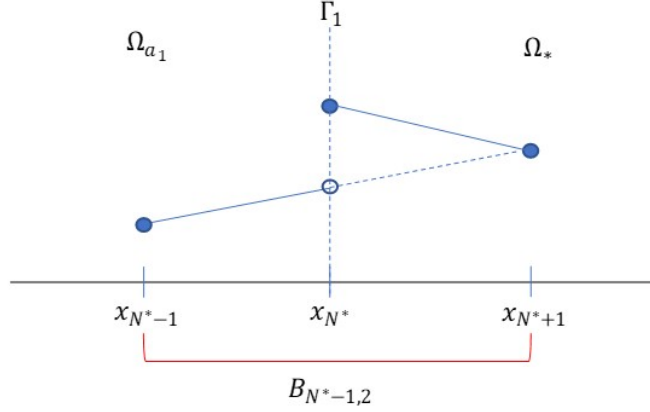
$$\frac{1}{\eta_1 \eta_2} \int_{B_{\ell, \eta}} \nabla v(x) \cdot \eta \, dx = \varepsilon (v_{\ell+\eta} - v_\ell), \quad (1.37)$$

and the lemma holds true.  $\square$

### 1.3.1 The discontinuous bond volume based coupling method

In this section we highlight how the *discontinuous coupled method* can be designed. The method, introduced in [19], allows flexibility on the construction of the underlying meshes and the computation of the energy at the interface is not involved. To retain consistency the interfacial energies should include terms accounting for the possible discontinuity of the underlying functions, and hence the name discontinuous coupling.

The design of the method is done with respect to the bond volumes  $B_{\ell, \eta}$ . Specifically, we consider three cases which are determined by the location of bond volume  $B_{\ell, \eta}$



**Figure 1.5:** An example of the bond  $B_{N^*-1,2}$  intersecting the interface  $\Gamma_1$ .

- a.  $\overline{B}_{\ell,\eta} \subset \Omega_a$ : The closure of bond volume  $\overline{B}_{\ell,\eta}$  is contained in  $\Omega_a$ ,
- b.  $B_{\ell,\eta} \subset \Omega_*$ : The bond volume  $\overline{B}_{\ell,\eta}$  is contained in region  $\Omega_*$ ,
- c.  $B_{\ell,\eta} \in B_\Gamma$  if it intersects the interface, i.e.  $\overline{B}_{\ell,\eta} \cap \Gamma \neq \emptyset$ .

In one dimension, if the bond has length 2 then there is one bond that intersects the interface and all the rest of the the bonds are either in the atomistic region  $\Omega_a$  or the atomistic Cauchy-Born region  $\Omega_*$  as displayed in Figure 1.5. If the bond has length 3 then there are two bonds that intersect the interface. In two dimensions, if the bond volume  $B_{\ell,\eta}$  has  $\eta = (2, 2)$  then there are  $4(N^{**} - N^* + 1)$  bond volumes that intersect the interface and all the others are in the atomistic region or the atomistic Cauchy-Born region as in Figure 1.6

The contribution to the energy which corresponds to a), for a fixed  $\eta$ , is:

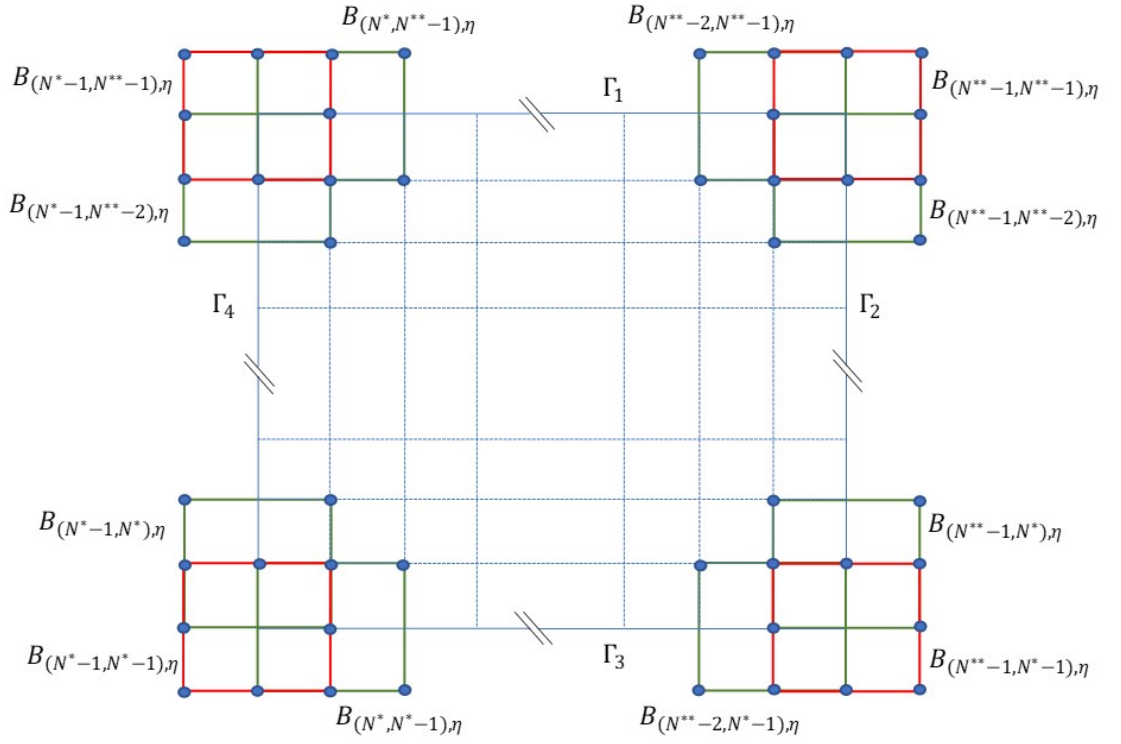
$$E_{\Omega_a,\eta}^a\{y\} = \varepsilon^2 \sum_{\substack{\ell \in \mathcal{L} \\ \overline{B}_{\ell,\eta} \subset \Omega_a}} \phi(\overline{D}_\eta y_\ell). \quad (1.38)$$

For a fixed  $\eta$ , the contribution to the energy which corresponds to the atomistic CB region is

$$E_{\Omega_*,\eta}^{a,cb}\{y\} = \sum_{K \subset \Omega_*} \phi(\nabla \overline{y}(m_K)\eta) = \int_{\Omega_*} \phi(\nabla \overline{y}(x)\eta) dx \quad (1.39)$$

where  $\overline{y}$  is the piecewise bilinear function at the lattice cells,  $\overline{y}^{\ell,\eta} \in \mathbb{Q}_1(K)$  interpolating  $\{y_\ell\}$ . Let  $y^{\ell,\eta}$  be a piecewise polynomial function on  $B_{\ell,\eta}$  for each bond volume  $B_{\ell,\eta}$  intersecting the interface  $\Gamma$  that satisfies

- i)  $y^{\ell,\eta} \in C(\overline{B_{\ell,\eta}} \setminus \Gamma)$ .
- ii) if  $B_{\ell,\eta} \cap \Gamma \neq \emptyset$  then  $y^{\ell,\eta}|_{\Omega_a} = \tilde{y}^{\ell,\eta}|_{\Omega_a}$  where  $\tilde{y}^{\ell,\eta} \in \mathbb{Q}_1(B_{\ell,\eta})$  is the bilinear function of  $B_{\ell,\eta}$  interpolating the values of  $y_\ell$  at the four vertices of  $B_{\ell,\eta}$ .
- iii) if  $B_{\ell,\eta} \cap \Gamma \neq \emptyset$  then  $y^{\ell,\eta}|_{\Omega_*} = \overline{y}^{\ell,\eta}|_{\Omega_*}$ , where, as above,  $\overline{y}$  is the piecewise bilinear function at the lattice cells  $K \subset B_{\ell,\eta} \cap \Omega_*$ ,  $\overline{y}^{\ell,\eta} \in \mathbb{Q}_1(K)$  interpolating  $\{y_\ell\}$ .



**Figure 1.6:** An example of the bond  $B_{N^*-1,2}$  intersecting the interface  $\Gamma_1$ .



**Figure 1.7:** (a) An example of  $y^{N*-2,3}$  on the bond  $B_{N*-2,3}$  that intersects interface  $\Gamma_1$ , (b) An example of  $y^{N*-1,3}$  on the bond  $B_{N*-1,3}$  that intersects interface  $\Gamma_1$ .

In one dimension, for  $\eta = 3$  there are only two bonds that intersect the interface,  $B_{N*-2,3}$  and  $B_{N*-1,3}$  as can be seen in Figure 1.7. For  $B_{N*-2,3}$ , in the atomistic region  $y^{\ell,\eta}$  is the interpolation of the values  $y_{N*-2}$  and  $y_{N*+1}$ , which are the end indices of the bond. In the atomistic Cauchy-Born region  $y^{\ell,\eta}$  is the interpolation of  $y_{N*+1}$  and  $y_{N*}$ . For  $B_{N*-1,3}$ , in the atomistic region  $y^{\ell,\eta}$  is the interpolation of the values  $y_{N*-1}$  and  $y_{N*+2}$ . In the atomistic Cauchy-Born region  $y^{\ell,\eta}$  is a piecewise linear function which is an interpolation of  $y_{N*+1}$  and  $y_{N*}$  in region  $[x_{N*}, x_{N*+1}]$  and an interpolation of  $y_{N*+2}$  and  $y_{N*+1}$  in region  $[x_{N*+1}, x_{N*+2}]$ .

Without entering into technical issues, we will define the energy at the interface following [19]. The energy for the bond volumes intersecting the interface can be defined as

$$E_{\Gamma,\eta}^D\{y\} = \sum_{\substack{\ell \in \mathcal{L} \\ B_{\ell,\eta} \in B_\Gamma}} \frac{1}{|\eta_1 \eta_2|} \left[ \int_{B_{\ell,\eta}} \chi_{\Omega_a} \phi(\nabla y^{\ell,\eta} \eta) dx - \int_{B_{\ell,\eta} \cap \Gamma} \phi'(\llbracket \nabla y^{\ell,\eta} \eta \rrbracket) \cdot \llbracket y^{\ell,\eta} \eta \rrbracket dS \right]. \quad (1.40)$$

Here,  $\llbracket w \eta \rrbracket$ , denotes the jump and  $\llbracket w \rrbracket$  denotes the average of a possibly discontinuous function on the interface

$$\llbracket w \eta \rrbracket := (\nu_{\Omega_a} \cdot \eta) w^- + (\nu_{\Omega_*} \cdot \eta) w^+, \quad \llbracket w \rrbracket := \frac{1}{2} \{w^- + w^+\}, \quad (1.41)$$

where  $w^-$  is the limit taken from  $\Omega_a$  and  $w^+$  is the limit taken from  $\Omega_*$ . Also,  $\nu_{\Omega_a}$  and  $\nu_{\Omega_*}$  are the respective exterior normal unit vectors, that satisfy  $\nu_{\Omega_a} = -\nu_{\Omega_*}$  on  $\Gamma$ . The last term in (1.40) is added to account for the loss of continuity of underlying functions, which seems to be the real source of inconsistency of first variations at the interface. In fact, when this term is not present Gauss-Green theorem yields a non-zero term at (1), which can be cancelled by adding the last term of (1.40) at the energy level. This account is explained in detail in [19].

The total energy is defined as

$$\mathcal{E}_{bv}\{y\} = \sum_{\eta \in R} \mathcal{E}_\eta\{y\}, \quad (1.42)$$

where

$$\mathcal{E}_\eta\{y\} = E_{\Omega_a,\eta}^a\{y\} + E_{\Omega_*,\eta}^{a,cb}\{y\} + E_{\Gamma,\eta}\{y\}. \quad (1.43)$$

Despite the fact that we allow discontinuities, the energy  $\mathcal{E}_{bv}^D$  is consistent (ghost-force free) [19].

**Proposition 1.** *The energy (1.42) is ghost force free, meaning that*

$$\langle D\mathcal{E}_{bv}^D(y_F), v \rangle = 0, \quad y_F(x) = \mathbf{F}x, \quad (1.44)$$

for all  $v \in \mathcal{V}$ .

### 1.3.2 Existing results and thesis outline

This thesis is devoted to the analysis and the construction of new energy based methods free of ghost forces in *two-dimensional crystal lattices* which are variants of the discontinuous coupled methods discussed in the previous section. Other approaches, which however are restricted to at most two dimensional lattices were proposed by Shapeev [29], see also [13]. Other works dealing with similar problems include [35, 11, 36, 5, 12, 28, 15, 30, 25, 26], see also [18] for a review. We will restrict our attention to pair potentials, allowing interactions of finite but otherwise arbitrarily long range.

In Chapter 2 we analyse the energy consistency of the discontinuous bond volume based coupled method in one dimension. In Chapter 3 we examine the variational consistency of the method in one dimension. The method considered is the natural restriction in one dimension of the method introduced in Section 1.3.1. These are the first error estimates in the literature for this method. They demonstrate its optimal analytical behaviour. Numerical experiments for two model problems are included in Chapter 3. Chapter 4 contains the analysis of the energy consistency of an adapted version of the discontinuous bond volume based coupled method in two dimensions. In Chapter 5 we examine the variational consistency of the method in two dimensions. Both chapters are devoted to a new method which emerged from the analysis in Chapter 5. The method, although similar in spirit to [19], since at the end we add discontinuous type terms at the interface to account for the inconsistency, has a different structure. The key idea is that without specifying the interface terms, our analysis leads to two types of terms: (a) terms which are  $O(\varepsilon^2)$  and vanish when  $y = y_F$  and (b) terms which are  $O(1)$  even for  $y = y_F$ . However, the terms in (b) are explicit and they have an appropriate structure which motivates the correct introduction of interface energy terms in order to eliminate their effect. The presentation is done in two dimensions and for  $\eta = (2, 2)$  in order to fix ideas and to simplify the complicated analysis and calculations. As is evident from [21] these results are applicable to general  $\eta$  and can be extended by similar, but tedious calculations to three dimensions. Furthermore, the error estimates of Chapters 4 and 5 are valid for the original version discontinuous bond volume coupled method, described in Section 1.3.1, see [19], with simple modifications in the analysis. The only other sharp analytical results for energy coupled methods in the literature can be found in [22, 24], and are restricted to two dimensions. Our analytical approach is entirely different. In fact the common theme of the present thesis is to extend the analytical approach introduced in [21] to derive estimates for coupled methods. This is a non-trivial task given the complications introduced by the presence of the interface between atomistic and continuum domains. As the ghost-force phenomenon appears only at the first variations level it is important to access the quality of the approximation of the coupled models both at the energy level (energy consistency) and at the first variation level (variational consistency). Chapters 2 and 4 are devoted to error estimates for the energies for one and two dimensions respectively.



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In Chapters 3 and 5 we prove error estimates for the first variations in one and two dimensions. Finally, in Chapter 6 we analyse the consistency of the atomistic versus the continuum model for multi-body potentials.

# Chapter 2

## Energy Consistency in 1D

### 2.1 Chapter Overview

In this chapter we will describe in detail the coupled method of Section 1.3.1 but restricting ourselves to one-dimension, and we will analyse the energy consistency of the method. We provide the definitions and notations that will be used in this chapter in Section 2.2. In Section 2.2.1 we introduce the atomistic potential energy for  $\eta = 2$  in (2.12) and in Section 2.2.2 we introduce the atomistic Cauchy-Born energy for  $\eta = 2$  in (2.17). In Section 2.2.3 we explain how we obtain the coupled energy corresponding on the two interfaces for  $\eta = 2$ . In Section 2.2.4 we state the coupled energy (2.33) and each of its components explicitly in (2.34). In Section 2.3 we take the difference between the coupled energy for  $\eta = 2$  and the atomistic Cauchy-Born energy and obtain (2.36). We can compare the coupled energy to the atomistic Cauchy-Born energy instead of the fully atomistic energy because the atomistic Cauchy-Born energy is a second order approximation to the fully atomistic energy, as explained in Chapter 1. We compared the coupled energy to the atomistic Cauchy-Born energy instead of comparing it to the fully atomistic energy because it is technically convenient to use this intermediate model in the analysis. Since the atomistic Cauchy-Born energy is composed of terms of the form  $\phi(2y'(m_K))$  for symmetry reasons we need to compare them with atomistic terms involving  $\phi(\overline{D}_2 y_\ell)$  and  $\phi(2\overline{D}_1 y_\ell)$  since

$$|\frac{1}{2}\overline{D}_2 y_\ell + \frac{1}{2}\overline{D}_2 y_{\ell+1} - 2y'(m_{\ell+1})| \leq O(\varepsilon^2),$$

see Lemmas 3-5. In Lemmas 3-4 we rearrange the sums in order to create symmetries as above. By using this type of symmetry we obtain in Lemma 3,

$$\begin{aligned} E_{\Omega_{a_1},2}^a\{y\} &= \varepsilon \sum_{\ell=1}^{N^*-2} \phi(\overline{D}_2 y_\ell) \\ &= \varepsilon \sum_{\ell=1}^{N^*-3} \phi(2y'(m_{\ell+1})) + \frac{\varepsilon}{2} [\phi(\overline{D}_2 y_1) + \phi(\overline{D}_2 y_{N^*-2})] + O(\varepsilon^2). \end{aligned}$$

so that when subtracted from the corresponding atomistic Cauchy-Born region what remains involves boundary terms of the form, see (2.58),

$$\varepsilon \phi(2y'(m_{(x_1,x_2)})) - \frac{\varepsilon}{2} [\phi(\overline{D}_2 y_1) + \phi(\overline{D}_2 y_{N^*-2})] + O(\varepsilon^2).$$

We apply Lemmas 3-5 to (2.36) and what remains are the interface terms and some bulk terms in (2.64). We then prove that the interface terms are second order. First, we apply Lemma 6 to get

$$|\phi' \left( \frac{y_{N^*+1} - y_{N^*-1}}{2\varepsilon} + \frac{y_{N^*+1} - y_{N^*}}{\varepsilon} \right) [y_{N^*-1} + y_{N^*+1} - 2y_{N^*}]| \leq O(\varepsilon^2),$$

and Lemma 7 to some terms close to the interface such that

$$|\varepsilon \phi(2y'(m_{N^*-1})) - \frac{\varepsilon}{2} \phi(\overline{D}_2 y_{N^*-2}) - \frac{\varepsilon}{2} \phi(\overline{D}_2 y_{N^*-1})| \leq O(\varepsilon^2).$$

Then the remaining bulk terms have the form

$$\varepsilon \phi(2y'(m_1)) - \frac{\varepsilon}{2} \phi(\overline{D}_2 y_1) - \frac{\varepsilon}{2} \phi(\overline{D}_2 y_N),$$

given in (2.76). By applying the periodicity condition these terms are also of order  $O(\varepsilon^2)$ . We conclude by proving Theorem 1 which shows that for a smooth function  $y$  the energy consistency error is of second order as follows

$$|\Phi_2^{CB}(y) - \mathcal{E}_2^D\{y\}| \leq O(\varepsilon^2).$$

Similar approach is taken for  $\eta = 3$  in Section 2.4 where we prove Theorem 2 which shows that for a smooth function  $y$  the energy consistency error is of second order as follows

$$|\Phi_3^{CB}(y) - \mathcal{E}_3^D\{y\}| \leq O(\varepsilon^2).$$

## 2.2 Definitions and Notation

Before any deformation, the material is in its reference state. The material will be represented as an equidistant number of atoms on a horizontal line with  $N$  number of atoms. The positions of the atoms on the line are the reference points  $x_\ell = \varepsilon \ell$ ,  $1 \leq \ell \leq N$  where  $\varepsilon$  is the distance between each atom in the reference state, i.e. the interatomic distance. Let

$$\mathcal{L} = \{\ell \mid 1 \leq \ell \leq N\}, \quad (2.1)$$

then the set of reference points can be denoted by

$$\Omega_{discr} = \{x_\ell = \varepsilon \ell, 1 \leq \ell \leq N\}, \quad N \in \mathbb{N}. \quad (2.2)$$

The atomistic deformations are expressed as discrete functions  $y_\ell = y(x_\ell)$ , such that

$$\begin{aligned} y_\ell &= Fx_\ell + v_\ell, \quad 1 \leq \ell \leq N \\ &= F\varepsilon \ell + v_\ell, \end{aligned} \quad (2.3)$$

where  $F$  is a constant with  $F > 0$  and  $v_\ell = v(x_\ell)$  is  $N$  periodic with respect to  $\mathcal{L}$  and has a zero average with respect to  $\mathcal{L}$ . Hence  $v_\ell$  satisfies

$$\begin{aligned} v_{\ell+N} &= v_\ell, \quad 1 \leq \ell \leq N, \\ \sum_{\ell=1}^N v_\ell &= 0. \end{aligned} \quad (2.4)$$

The atomistic deformations  $y_\ell$ , satisfy

$$\begin{aligned} y_{\ell+N} &= Fx_{\ell+N} + v_{\ell+N} \\ &= F\varepsilon(\ell + N) + v_{\ell+N} \\ &= F\varepsilon\ell + F\varepsilon N + v_\ell \\ &= y_\ell + F\varepsilon N, \end{aligned} \tag{2.5}$$

where (2.3) and (2.4) have been utilised. Therefore,

$$y_{\ell+N} = y_\ell + F\varepsilon N, \quad 1 \leq \ell \leq N. \tag{2.6}$$

The atomistic deformations  $y_\ell$  also satisfy

$$\begin{aligned} y_{\ell+1+N} - y_{\ell+N} &= F\varepsilon(\ell + 1 + N) + v_{\ell+1+N} - F\varepsilon(\ell + N) - v_{\ell+N} \\ &= F\varepsilon + v_{\ell+1+N} - v_{\ell+N} \\ &= F\varepsilon + v_{\ell+1} - v_\ell \\ &= F\varepsilon(\ell + 1) + v_{\ell+1} - F\varepsilon\ell - v_\ell \\ &= y_{\ell+1} - y_\ell. \end{aligned} \tag{2.7}$$

Therefore,

$$y_{\ell+1+N} - y_{\ell+N} = y_{\ell+1} - y_\ell, \quad 1 \leq \ell \leq N. \tag{2.8}$$

### 2.2.1 Atomistic potential energy

The atomistic potential is

$$\Phi^\alpha(y) = \varepsilon \sum_{\ell=1}^N \sum_{\eta=-N_R}^{N_R} \phi\left(\frac{y_{\ell+\eta} - y_\ell}{\varepsilon}\right), \tag{2.9}$$

where  $\eta \in \mathbb{Z}$  and  $N_R \in \mathbb{N}$  is the number of neighbour atoms that atom  $\ell$  interacts with. We assume that the short range interactions of the atoms are approximated by the pair potential (usually the Lennard-Jones potential or the Morse potential). The discrete derivative in the direction of the constant  $\eta \in \mathbb{Z}$  is defined as

$$\overline{D}_\eta y_\ell = \frac{y_{\ell+\eta} - y_\ell}{\varepsilon}, \quad \ell \in \mathcal{L}, \tag{2.10}$$

and so the atomistic potential in equation (2.9) can be written as

$$\Phi^\alpha(y) = \varepsilon \sum_{\ell=1}^N \sum_{\eta=-N_R}^{N_R} \phi(\overline{D}_\eta y_\ell). \tag{2.11}$$

As mentioned in Chapter 1, we do not assume any symmetry for the potential  $\phi$  except in Chapter 6. For the rest of Section 2.2 and Section 2.3 we will fix  $\eta = 2$  since the analysis suggests that we can work for each  $\eta = -N_R, \dots, N_R$ , separately. We chose  $\eta = 2$  since this is the simplest case where inconsistency on the interface may occur. Let us consider the case that  $\eta = 2$ , then the atomistic potential energy, equation (2.11) is

$$\Phi_2^\alpha(y) = \varepsilon \sum_{\ell=1}^N \phi(\overline{D}_2 y_\ell). \tag{2.12}$$

since  $\eta$  is fixed and we are looking at the next nearest neighbours to the right of the atom. The reason why  $\eta = 1$  is not considered will be explained in Section 2.2.3.

### 2.2.2 Continuum Cauchy-Born potential energy for $\eta = 2$

Let

$$T = \{K \subset \Omega : K = (x_\ell, x_{\ell+1}), \quad \Omega = [x_1, x_{N+1}]\}, \quad (2.13)$$

and let  $m_K$  denote the middle point of  $K$ . The continuum Cauchy-Born potential energy is

$$\Phi^{CB}(y) = \int_{\Omega} W_{CB}(y'(x)) dx = \sum_{K \in T} \int_K W_{CB}(y'(x)) dx, \quad (2.14)$$

where

$$W_{CB}(y'(x)) = \sum_{\eta \in R} \phi(y'(x)\eta). \quad (2.15)$$

A second order approximation of the Cauchy-Born energy is the atomistic Cauchy-Born energy, [21],

$$\Phi^{a,CB}(y) = \varepsilon \sum_{K \in T} W_{CB}(y'(m_K)). \quad (2.16)$$

In the case where  $\eta = 2$ , it is reduced to

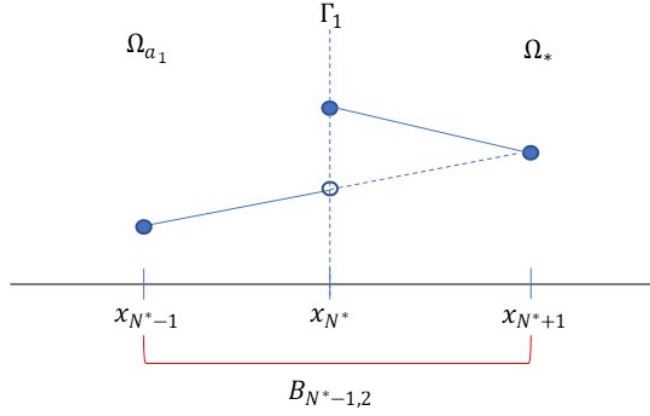
$$\begin{aligned} \Phi_2^{a,CB}(y) = \varepsilon \sum_{K \in T} \phi(2y'(m_K)) = & \varepsilon [\phi(2y'(m_{(x_1, x_2)})) + \phi(2y'(m_{(x_2, x_3)})) + \cdots \\ & + \phi(2y'(m_{(x_N, x_{N+1})}))]. \end{aligned} \quad (2.17)$$

### 2.2.3 Energy on the interfaces for $\eta = 2$

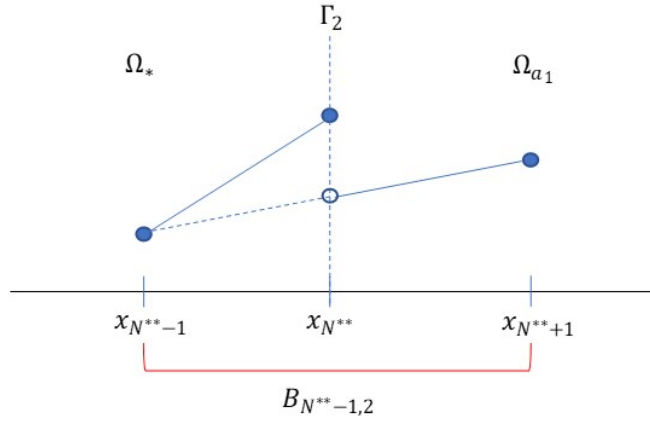
The idea for the discontinuous bond volume based coupling method was described in Section 1.3.1 of Chapter 1. The reason why we do not consider  $\eta = 1$  is that the bond volume cannot intersect with the interface, it is like a unit cell and it will either exist in the atomistic region or in the atomistic Cauchy-Born region. Therefore there is no energy on the interface for bond volumes with  $\eta = 1$ . We split the domain  $\Omega$  into three regions,  $\Omega_{a_1} = [x_1, x_{N^*})$ ,  $\Omega_* = (x_{N^*}, x_{N^{**}})$  and  $\Omega_{a_2} = [x_{N^{**}}, x_{N+1}]$ , where  $\Omega_{a_1}$  and  $\Omega_{a_2}$  are atomistic regions and  $\Omega_*$  is the atomistic Cauchy-Born region.  $\Gamma_1 = x_{N^*}$  is the interface between  $\Omega_{a_1}$  and  $\Omega_*$ , and  $\Gamma_2 = x_{N^{**}}$  is the interface between  $\Omega_*$  and  $\Omega_{a_2}$ , where  $1 < N^* < N^{**} < N$ , as in Figure 2.3. The bond  $B_{\ell,2}$ , already described in section 1.3 of Chapter 1 that intersects the interface  $\Gamma_1$  is  $B_{N^*-1,2}$  and the bond that intersects with interface  $\Gamma_2$  is  $B_{N^{**}-1,2}$ . Let  $\bar{B}_{N^*-1,2} = [x_{N^*-1}, x_{N^*}] \cup [x_{N^*}, x_{N^*+1}]$  where  $x_{N^*}$  is on interface  $\Gamma_1$ . Let  $y^{\ell,2}$  be the continuous, piecewise linear function on the bond  $B_{\ell,2} = [x_\ell, x_{\ell+2}]$  that intersects an interface, such that  $y^{\ell,2}$  is linear on  $(x_\ell, x_{\ell+1})$  and linear on  $(x_{\ell+1}, x_{\ell+2})$ . For  $\Gamma_1$ ,  $y^{N^*-1,2}$  is linear on  $(x_{N^*-1}, x_{N^*})$  and linear on  $(x_{N^*}, x_{N^*+1})$ , as shown in Figure 2.1. For  $\Gamma_2$ ,  $y^{N^{**}-1,2}$  is linear on  $(x_{N^{**}-1}, x_{N^{**}})$  and linear on  $(x_{N^{**}}, x_{N^{**}+1})$ , as shown in Figure 2.2. For  $\Gamma_1$ , let  $y^{N^*-1,2-}$  and  $y^{N^*-1,2+}$  be the limits taken from  $\Omega_{a_1}$  and  $\Omega_*$  respectively as follows

$$y^{N^*-1,2+}(x) = y_{N^*} \quad (2.18)$$

$$y^{N^*-1,2-}(x) = y_{N^*-1} + \left( \frac{y_{N^*+1} - y_{N^*-1}}{2\varepsilon} \right) (x - x_{N^*-1}). \quad (2.19)$$



**Figure 2.1:** An example of  $y^{N^*-1,2}$  on the bond  $B_{N^*-1,2}$  that intersects interface  $\Gamma_1$ .



**Figure 2.2:** An example of  $y^{N^{**}-1,2}$  on the bond  $B_{N^{**}-1,2}$  that intersects interface  $\Gamma_2$ .

Their corresponding derivatives are

$$(y^{N^*-1,2})'^+(x_{N^*}) = \frac{y_{N^*+1} - y_{N^*}}{\varepsilon} \quad (2.20)$$

$$(y^{N^*-1,2})'^-(x_{N^*}) = \frac{y_{N^*+1} - y_{N^*-1}}{2\varepsilon}. \quad (2.21)$$

For  $\Gamma_2$ , let  $y^{N^{**}-1,2-}$  and  $y^{N^{**}-1,2+}$  be the limits taken from  $\Omega_*$  and  $\Omega_{a_2}$  respectively such that

$$y^{N^{**}-1,2+}(x) = y_{N^{**}-1} + \left( \frac{y_{N^{**}+1} - y_{N^{**}-1}}{2\varepsilon} \right) (x - x_{N^{**}-1}) \quad (2.22)$$

$$y^{N^{**}-1,2-}(x) = y_{N^{**}}. \quad (2.23)$$

Their corresponding derivatives are

$$(y^{N^{**}-1,2})'^+(x_{N^{**}}) = \frac{y_{N^{**}+1} - y_{N^{**}-1}}{2\varepsilon} \quad (2.24)$$

$$(y^{N^{**}-1,2})'^-(x_{N^{**}}) = \frac{y_{N^{**}} - y_{N^{**}-1}}{\varepsilon}. \quad (2.25)$$

The form of the energy is the same for both interfaces  $\Gamma_1$  and  $\Gamma_2$  and so for simplicity we will define the energy for a general  $\Gamma$ . The energy for the bond volumes intersecting the interface is defined in 1.40. We first calculate the first term of 1.40 as follows

$$\sum_{\substack{\ell \in \mathcal{L} \\ B_{\ell,2} \cap \Gamma \neq \emptyset}} \frac{1}{2} \int_{B_{\ell,2}} \chi_{\Omega_a} \phi(2(y^{\ell,2})') dx = \sum_{\substack{\ell \in \mathcal{L} \\ B_{\ell,2} \cap \Gamma \neq \emptyset}} \frac{1}{2} \varepsilon \phi\left(2 \frac{y_{\ell+2} - y_{\ell}}{2\varepsilon}\right) = \varepsilon \sum_{\substack{\ell \in \mathcal{L} \\ B_{\ell,2} \cap \Gamma \neq \emptyset}} \frac{1}{2} \phi(\bar{D}_2 y_{\ell}). \quad (2.26)$$

The method, described in Section 1.3.1, allows discontinuous matching across the interface  $\Gamma$ , the energy due to bonds intersecting the interface is

$$\begin{aligned} E_{\Gamma,2}^D\{y\} &= \sum_{\substack{\ell \in \mathcal{L} \\ B_{\ell,2} \cap \Gamma \neq \emptyset}} \frac{1}{2} \left[ \int_{B_{\ell,2}} \chi_{\Omega_a} \phi(2(y^{\ell,2})') dx - \int_{B_{\ell,2} \cap \Gamma} \phi'(\{2(y^{\ell,2})'\}) \cdot \llbracket 2y^{\ell,2} \rrbracket dS \right] \\ &= \frac{1}{2} \left[ \sum_{\substack{\ell \in \mathcal{L} \\ B_{\ell,2} \cap \Gamma \neq \emptyset}} \varepsilon \phi(\bar{D}_2 y_{\ell}) - \phi'(\{2(y^{\ell,2}(x_{\ell+1}))'\}) \llbracket 2y^{\ell,2}(x_{\ell+1}) \rrbracket \right] \\ &= \frac{1}{2} \left[ \sum_{\substack{\ell \in \mathcal{L} \\ B_{\ell,2} \cap \Gamma \neq \emptyset}} \varepsilon \phi(\bar{D}_2 y_{\ell}) - \phi'\left(\frac{1}{2}\{2(y^{\ell,2})'^- + 2(y^{\ell,2})'^+\}\right) [2(y^{\ell,2})^+ - 2(y^{\ell,2})^-] \right]. \end{aligned} \quad (2.27)$$

Here,  $\llbracket w \rrbracket$ ,  $\{w\}$  denote the jump and the average of a possibly discontinuous function on the interface

$$\llbracket w \rrbracket := \eta w^- - \eta w^+ \quad (2.28)$$

$$\{w\} := \frac{1}{2}\{w^- + w^+\} \quad (2.29)$$

$w^-$  and  $w^+$  being the limits taken from  $\Omega_a$  and  $\Omega_*$  respectively. Now, we define the interface energy terms at  $\Gamma_1$  and  $\Gamma_2$ . The only bond  $B_{\ell,2}$  that intersects the interface  $\Gamma_1$  is  $B_{N^*-1,2}$  and hence

$$\begin{aligned} E_{\Gamma_1,2}^D\{y\} &= \frac{\varepsilon}{2} \phi(\bar{D}_2 y_{N^*-1}) \\ &\quad - \frac{1}{2} \phi'(\{(y^{N^*-1,2})'^- + (y^{N^*-1,2})'^+\}) [2(y^{N^*-1,2})^- - 2(y^{N^*-1,2})^+] \\ &= \frac{\varepsilon}{2} \phi(\bar{D}_2 y_{N^*-1}) - \frac{1}{2} \phi'\left(\frac{y_{N^*+1} - y_{N^*-1}}{2\varepsilon} + \frac{y_{N^*+1} - y_{N^*}}{\varepsilon}\right) [2y_{N^*-1} \\ &\quad + 2\left(\frac{y_{N^*+1} - y_{N^*-1}}{2\varepsilon}\right)(x_{N^*} - x_{N^*-1}) - 2y_{N^*}] \\ &= \frac{\varepsilon}{2} \phi(\bar{D}_2 y_{N^*-1}) \\ &\quad - \frac{1}{2} \phi'\left(\frac{y_{N^*+1} - y_{N^*-1}}{2\varepsilon} + \frac{y_{N^*+1} - y_{N^*}}{\varepsilon}\right) [y_{N^*-1} + y_{N^*+1} - 2y_{N^*}]. \end{aligned} \quad (2.30)$$

The only bond  $B_{\ell,2}$  that intersects the interface  $\Gamma_2$  is  $B_{N^{**}-1,2}$  and hence

$$\begin{aligned}
E_{\Gamma_2,2}^D\{y\} &= \frac{\varepsilon}{2}\phi(\overline{D}_2 y_{N^{**}-1}) \\
&\quad - \frac{1}{2}\phi'(\mathbb{I}(y^{N^{**}-1,2})'^- + (y^{N^{**}-1,2})'^+)[2(y^{N^{**}-1,2})^- - 2(y^{N^{**}-1,2})^+] \\
&= \frac{\varepsilon}{2}\phi(\overline{D}_2 y_{N^{**}-1}) - \frac{1}{2}\phi'\left(\frac{y_{N^{**}} - y_{N^{**}-1}}{\varepsilon} + \frac{y_{N^{**}+1} - y_{N^{**}-1}}{2\varepsilon}\right)[2y_{N^{**}} \\
&\quad - 2y_{N^{**}-1} - 2\left(\frac{y_{N^{**}+1} - y_{N^{**}-1}}{2\varepsilon}\right)(x_{N^{**}} - x_{N^{**}-1})] \\
&= \frac{\varepsilon}{2}\phi(\overline{D}_2 y_{N^{**}-1}) \\
&\quad - \frac{1}{2}\phi'\left(\frac{y_{N^{**}} - y_{N^{**}-1}}{\varepsilon} + \frac{y_{N^{**}+1} - y_{N^{**}-1}}{2\varepsilon}\right)[2y_{N^{**}} - y_{N^{**}-1} - y_{N^{**}+1}].
\end{aligned} \tag{2.31}$$

### 2.2.4 Atomistic to Continuum Coupled Energy for $\eta = 2$

We define the total coupling energy as:

$$\mathcal{E}_{bv}^D\{y\} = \sum_{\eta \in R} \mathcal{E}_{\eta}^D\{y\}, \tag{2.32}$$

where

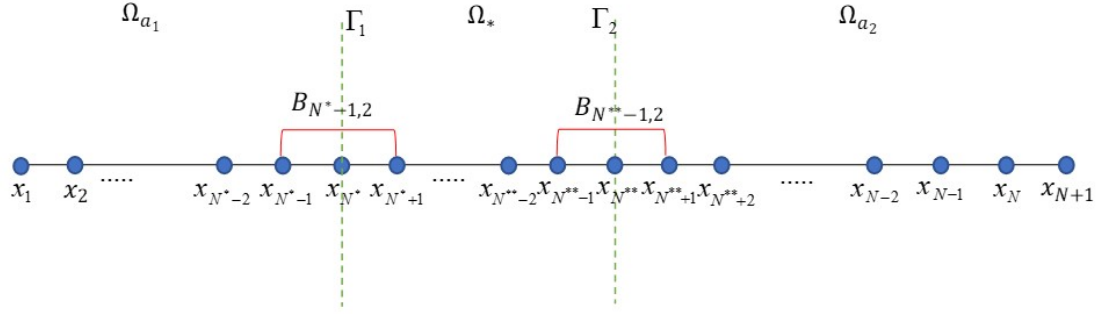
$$\mathcal{E}_{\eta}^D\{y\} = E_{\Omega_{a_1},\eta}^a\{y\} + E_{\Gamma_1,\eta}^D\{y\} + E_{\Omega_*,\eta}^{a,CB}\{y\} + E_{\Gamma_2,\eta}^D\{y\} + E_{\Omega_{a_2},\eta}^a\{y\}. \tag{2.33}$$

Here,  $\Omega_{a_1}$  and  $\Omega_{a_2}$  are the atomistic regions while  $\Omega_*$  is the atomistic Cauchy-Born region.

For fixed  $\eta = 2$ ,

$$\begin{aligned}
E_{\Omega_{a_1},2}^a\{y\} &= \varepsilon \sum_{\ell=1}^{N^*-2} \phi(\overline{D}_2 y_{\ell}) \\
E_{\Gamma_1,2}^D\{y\} &= \frac{\varepsilon}{2}\phi(\overline{D}_2 y_{N^*-1}) - \frac{1}{2}\phi'\left(\frac{y_{N^*+1} - y_{N^*-1}}{2\varepsilon} + \frac{y_{N^*+1} - y_{N^*}}{\varepsilon}\right) \\
&\quad [y_{N^*-1} + y_{N^*+1} - 2y_{N^*}] \\
E_{\Omega_*,2}^{a,CB}\{y\} &= \varepsilon \sum_{\ell=N^*}^{N^{**}-1} \phi(2\overline{D}_1 y_{\ell}) \\
E_{\Gamma_2,2}^D\{y\} &= \frac{\varepsilon}{2}\phi(\overline{D}_2 y_{N^{**}-1}) - \frac{1}{2}\phi'\left(\frac{y_{N^{**}} - y_{N^{**}-1}}{\varepsilon} + \frac{y_{N^{**}+1} - y_{N^{**}-1}}{2\varepsilon}\right) \\
&\quad [2y_{N^{**}} - y_{N^{**}-1} - y_{N^{**}+1}] \\
E_{\Omega_{a_2},2}^a\{y\} &= \varepsilon \sum_{\ell=N^{**}}^N \phi(\overline{D}_2 y_{\ell}).
\end{aligned} \tag{2.34}$$





**Figure 2.3:** The atomistic to continuum coupling domain.

## 2.3 Comparison of coupled energy with continuum energy for $\eta = 2$

We split the atomistic Cauchy-Born energy to correspond to the domains of (2.34) as follows

$$\begin{aligned}
 \Phi_2^{a,CB}(y) = & \varepsilon \sum_{K=(x_1, x_2)}^{(x_{N^*-2}, x_{N^*-1})} \phi(2y'(m_K)) + \varepsilon \sum_{K=(x_{N^*-1}, x_{N^*})}^{(x_{N^*}, x_{N^*+1})} \phi(2y'(m_K)) \\
 & + \varepsilon \sum_{K=(x_{N^*+1}, x_{N^*+2})}^{(x_{N^{**}-2}, x_{N^{**}-1})} \phi(2y'(m_K)) + \varepsilon \sum_{K=(x_{N^{**}-1}, x_{N^{**}})}^{(x_{N^{**}}, x_{N^{**}+1})} \phi(2y'(m_K)) \\
 & + \varepsilon \sum_{K=(x_{N^{**}+1}, x_{N^{**}+2})}^{(x_N, x_{N+1})} \phi(2y'(m_K)) \\
 =: & A_{CB} + B_{CB} + \Gamma_{CB} + D_{CB} + G_{CB}.
 \end{aligned} \tag{2.35}$$

We will compute the error  $\Phi_2^{a,CB}(y) - \mathcal{E}_2^D\{y\}$  as follows

$$\begin{aligned}
\Phi_2^{a,CB}(y) - \mathcal{E}_2^D\{y\} &= A_{CB} - E_{\Omega_{a_1},2}^a\{y\} + B_{CB} - E_{\Gamma_{1,2}}^D\{y\} + \Gamma_{CB} - E_{\Omega_{a_2},2}^{a,CB}\{y\} \\
&\quad + D_{CB} - E_{\Gamma_{2,2}}^D\{y\} + G_{CB} - E_{\Omega_{a_2},2}^a\{y\} \\
&= \varepsilon \sum_{K=(x_1,x_2)}^{(x_{N^*-2},x_{N^*-1})} \phi(2y'(m_K)) - \varepsilon \sum_{\ell=1}^{N^*-2} \phi(\bar{D}_2 y_\ell) \\
&\quad + \varepsilon \sum_{K=(x_{N^*-1},x_{N^*})}^{(x_{N^*},x_{N^*+1})} \phi(2y'(m_K)) - \frac{\varepsilon}{2} \phi(\bar{D}_2 y_{N^*-1}) \\
&\quad + \frac{1}{2} \phi' \left( \frac{y_{N^*+1} - y_{N^*-1}}{x_{N^*+1} - x_{N^*-1}} + \frac{y_{N^*+1} - y_{N^*}}{\varepsilon} \right) [y_{N^*-1} + y_{N^*+1} - 2y_{N^*}] \\
&\quad + \varepsilon \sum_{K=(x_{N^*+1},x_{N^*+2})}^{(x_{N^*+2},x_{N^*+3})} \phi(2y'(m_K)) - \varepsilon \sum_{\ell=N^*}^{N^{**}-1} \phi(2\bar{D}_1 y_\ell) \\
&\quad + \varepsilon \sum_{K=(x_{N^*+1},x_{N^*+2})}^{(x_{N^*+2},x_{N^*+3})} \phi(2y'(m_K)) - \frac{\varepsilon}{2} \phi(\bar{D}_2 y_{N^*+1}) \\
&\quad + \frac{1}{2} \phi' \left( \frac{y_{N^*+2} - y_{N^*+1}}{\varepsilon} + \frac{y_{N^*+2} - y_{N^*+1}}{2\varepsilon} \right) [2y_{N^*+1} - y_{N^*+2} \\
&\quad - y_{N^*+3}] + \varepsilon \sum_{K=(x_{N^*+1},x_{N^*+2})}^{(x_N,x_{N+1})} \phi(2y'(m_K)) - \varepsilon \sum_{\ell=N^*}^N \phi(\bar{D}_2 y_\ell).
\end{aligned} \tag{2.36}$$

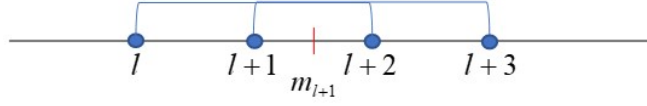
Below we introduce three lemmas that we will apply to (2.36).

**Lemma 3.** *For a smooth function  $y$  and a smooth function  $\phi$  whose derivatives are bounded we have*

$$\begin{aligned}
E_{\Omega_{a_1},2}^a\{y\} &= \varepsilon \sum_{\ell=1}^{N^*-2} \phi(\bar{D}_2 y_\ell) \\
&= \varepsilon \sum_{\ell=1}^{N^*-3} \phi(2y'(m_{\ell+1})) + \frac{\varepsilon}{2} [\phi(\bar{D}_2 y_1) + \phi(\bar{D}_2 y_{N^*-2})] + O(\varepsilon^2).
\end{aligned} \tag{2.37}$$

*Proof.* We will start by looking at  $E_{\Omega_{a_1},2}^a\{y\}$  and we will introduce the following symmetry splitting

$$\begin{aligned}
E_{\Omega_{a_1},2}^a\{y\} &= \varepsilon \sum_{\ell=1}^{N^*-2} \phi(\bar{D}_2 y_\ell) \\
&= \varepsilon \left\{ \frac{1}{2} \phi(\bar{D}_2 y_1) + \frac{1}{2} [\phi(\bar{D}_2 y_1) + \phi(\bar{D}_2 y_2)] + \frac{1}{2} [\phi(\bar{D}_2 y_2) + \phi(\bar{D}_2 y_3)] \right. \\
&\quad \left. + \cdots + \frac{1}{2} [\phi(\bar{D}_2 y_{N^*-3}) + \phi(\bar{D}_2 y_{N^*-2})] + \frac{1}{2} \phi(\bar{D}_2 y_{N^*-2}) \right\}.
\end{aligned} \tag{2.38}$$

**Figure 2.4:** Displaying  $m_{\ell+1}$ 

Therefore,

$$\varepsilon \sum_{\ell=1}^{N^*-2} \phi(\bar{D}_2 y_\ell) = \varepsilon \sum_{\ell=1}^{N^*-3} \frac{1}{2} [\phi(\bar{D}_2 y_\ell) + \phi(\bar{D}_2 y_{\ell+1})] + \frac{\varepsilon}{2} [\phi(\bar{D}_2 y_1) + \phi(\bar{D}_2 y_{N^*-2})]. \quad (2.39)$$

Let  $m_{\ell+1}$  denote the middle point between  $x_{\ell+1}$  and  $x_{\ell+2}$ , Figure 2.4. Obviously,

$$\begin{aligned} \bar{D}_2 y_\ell + \bar{D}_2 y_{\ell+1} &= \frac{y_{\ell+2} - y_\ell}{\varepsilon} + \frac{y_{\ell+3} - y_{\ell+1}}{\varepsilon} \\ &= \frac{y_{\ell+3} - y_\ell}{\varepsilon} + \frac{y_{\ell+2} - y_{\ell+1}}{\varepsilon} \\ &= 3y'(m_{\ell+1}) + y'(m_{\ell+1}) + O(\varepsilon^2) \\ &= 4y'(m_{\ell+1}) + O(\varepsilon^2), \end{aligned} \quad (2.40)$$

and hence,

$$\frac{1}{2} (\bar{D}_2 y_\ell + \bar{D}_2 y_{\ell+1}) = 2y'(m_{\ell+1}) + O(\varepsilon^2). \quad (2.41)$$

Since we have assumed that  $\phi$  is smooth (Assumption 1) and that its derivatives are bounded (Assumption 3) we can expand  $\phi(a)$  and  $\phi(b)$ , using Taylor expansion, around  $\left(\frac{a+b}{2}\right)$  and we obtain

$$\begin{aligned} \phi(a) &= \phi\left(\frac{a+b}{2}\right) - \phi'\left(\frac{a+b}{2}\right)\left(\frac{b-a}{2}\right) + \frac{1}{2}\phi''(\xi_1)\left(\frac{b-a}{2}\right)^2, \\ \phi(b) &= \phi\left(\frac{a+b}{2}\right) + \phi'\left(\frac{a+b}{2}\right)\left(\frac{b-a}{2}\right) + \frac{1}{2}\phi''(\xi_2)\left(\frac{b-a}{2}\right)^2. \end{aligned}$$

where  $\xi_1 \in \left(a, \frac{a+b}{2}\right)$  and  $\xi_2 \in \left(\frac{a+b}{2}, b\right)$ . Adding  $\phi(a)$  and  $\phi(b)$  yields

$$\left| \frac{\phi(a) + \phi(b)}{2} - \phi\left(\frac{a+b}{2}\right) \right| \leq c|a-b|^2. \quad (2.42)$$

By applying (2.42) in our case yields

$$\left| \frac{\phi(\bar{D}_2 y_\ell) + \phi(\bar{D}_2 y_{\ell+1})}{2} - \phi\left(\frac{\bar{D}_2 y_\ell + \bar{D}_2 y_{\ell+1}}{2}\right) \right| \leq c|\bar{D}_2 y_\ell - \bar{D}_2 y_{\ell+1}|^2 \leq c\varepsilon^2. \quad (2.43)$$

If we use the Taylor expansion of  $\phi\left(\frac{\bar{D}_2 y_\ell + \bar{D}_2 y_{\ell+1}}{2}\right)$  around  $2y'(m_{\ell+1})$  we get

$$\phi\left(\frac{\bar{D}_2 y_\ell + \bar{D}_2 y_{\ell+1}}{2}\right) = \phi(2y'(m_{\ell+1})) + \phi'(\xi) \left[ \frac{\bar{D}_2 y_\ell + \bar{D}_2 y_{\ell+1}}{2} - 2y'(m_{\ell+1}) \right], \quad (2.44)$$

where  $\xi$  is between  $\left(\frac{\bar{D}_2 y_\ell + \bar{D}_2 y_{\ell+1}}{2}\right)$  and  $2y'(m_{\ell+1})$ .

Hence, (2.44) implies,

$$\begin{aligned} \left| \phi\left(\frac{\bar{D}_2 y_\ell + \bar{D}_2 y_{\ell+1}}{2}\right) - \phi(2y'(m_{\ell+1})) \right| &\leq \left| \phi'(\xi) \left[ \frac{\bar{D}_2 y_\ell + \bar{D}_2 y_{\ell+1}}{2} - 2y'(m_{\ell+1}) \right] \right| \\ &\leq \max_{\xi} |\phi'(\xi)| \left| \frac{\bar{D}_2 y_\ell + \bar{D}_2 y_{\ell+1}}{2} - 2y'(m_{\ell+1}) \right| \\ &\leq c\varepsilon^2, \quad c \in \mathbb{R}. \end{aligned} \quad (2.45)$$

Therefore, (2.37) holds.  $\square$

**Lemma 4.** *For a smooth function  $y$  and a smooth function  $\phi$  whose derivatives are bounded we have*

$$\begin{aligned} E_{\Omega_{a_2}, 2}^a\{y\} &= \varepsilon \sum_{\ell=N^{**}}^N \phi(\bar{D}_2 y_\ell) \\ &= \varepsilon \sum_{\ell=N^{**}}^{N-1} \phi(2y'(m_{\ell+1})) + \frac{\varepsilon}{2} [\phi(\bar{D}_2 y_{N^{**}}) + \phi(\bar{D}_2 y_N)] + O(\varepsilon^2). \end{aligned} \quad (2.46)$$

*Proof.* The proof is very similar to Lemma 3. We will start by looking at  $E_{\Omega_{a_2}, 2}^a\{y\}$  and we will introduce the following symmetry splitting

$$\begin{aligned} E_{\Omega_{a_2}, 2}^a\{y\} &= \varepsilon \sum_{\ell=N^{**}}^N \phi(\bar{D}_2 y_\ell) \\ &= \varepsilon \left\{ \frac{1}{2} \phi(\bar{D}_2 y_{N^{**}}) + \frac{1}{2} [\phi(\bar{D}_2 y_{N^{**}}) + \phi(\bar{D}_2 y_{N^{**}+1})] \right. \\ &\quad + \frac{1}{2} [\phi(\bar{D}_2 y_{N^{**}+1}) + \phi(\bar{D}_2 y_{N^{**}+2})] + \cdots \\ &\quad \left. + \frac{1}{2} [\phi(\bar{D}_2 y_{N-1}) + \phi(\bar{D}_2 y_N)] + \frac{1}{2} \phi(\bar{D}_2 y_N) \right\}. \end{aligned} \quad (2.47)$$

Therefore,

$$\varepsilon \sum_{\ell=N^{**}}^N \phi(\bar{D}_2 y_\ell) = \varepsilon \sum_{\ell=N^{**}}^{N-1} \frac{1}{2} [\phi(\bar{D}_2 y_\ell) + \phi(\bar{D}_2 y_{\ell+1})] + \frac{\varepsilon}{2} [\phi(\bar{D}_2 y_{N^{**}}) + \phi(\bar{D}_2 y_N)]. \quad (2.48)$$

Let  $m_\ell$  denote the middle point between  $x_\ell$  and  $x_{\ell+1}$ . Using (2.40) we obtain

$$\frac{1}{2}(\overline{D}_2 y_\ell + \overline{D}_2 y_{\ell+1}) = 2y'(m_{\ell+1}) + O(\varepsilon^2). \quad (2.49)$$

As before, using

$$\left| \frac{\phi(a) + \phi(b)}{2} - \phi\left(\frac{a+b}{2}\right) \right| \leq c|a-b|^2, \quad (2.50)$$

we obtain

$$\left| \frac{\phi(\overline{D}_2 y_\ell) + \phi(\overline{D}_2 y_{\ell+1})}{2} - \phi\left(\frac{\overline{D}_2 y_\ell + \overline{D}_2 y_{\ell+1}}{2}\right) \right| \leq c\varepsilon^2. \quad (2.51)$$

If we use the Taylor expansion of  $\phi\left(\frac{\overline{D}_2 y_\ell + \overline{D}_2 y_{\ell+1}}{2}\right)$  around  $2y'(m_{\ell+1})$  then

$$\phi\left(\frac{\overline{D}_2 y_\ell + \overline{D}_2 y_{\ell+1}}{2}\right) = \phi(2y'(m_{\ell+1})) + \phi'(\xi) \left[ \frac{\overline{D}_2 y_\ell + \overline{D}_2 y_{\ell+1}}{2} - 2y'(m_{\ell+1}) \right], \quad (2.52)$$

where  $\xi$  is between  $\frac{\overline{D}_2 y_\ell + \overline{D}_2 y_{\ell+1}}{2}$  and  $2y'(m_{\ell+1})$ .

Hence,

$$\begin{aligned} \left| \phi\left(\frac{\overline{D}_2 y_\ell + \overline{D}_2 y_{\ell+1}}{2}\right) - \phi(2y'(m_{\ell+1})) \right| &\leq \left| \phi'(\xi) \left[ \frac{\overline{D}_2 y_\ell + \overline{D}_2 y_{\ell+1}}{2} - 2y'(m_{\ell+1}) \right] \right| \\ &\leq \max_{\xi} |\phi'(\xi)| \left| \frac{\overline{D}_2 y_\ell + \overline{D}_2 y_{\ell+1}}{2} - 2y'(m_{\ell+1}) \right| \\ &\leq c\varepsilon^2, \quad c \in \mathbb{R}. \end{aligned} \quad (2.53)$$

The proof is complete.  $\square$

**Lemma 5.** *For a smooth function  $y$  and a smooth function  $\phi$  whose derivatives are bounded we have*

$$E_{\Omega^*,2}^{a,CB}\{y\} = \varepsilon \sum_{\ell=N^*}^{N^{**}-1} \phi(2\overline{D}_1 y_\ell) = \varepsilon \sum_{\ell=N^*}^{N^{**}-1} \phi(2y'(m_\ell)) + O(\varepsilon^2). \quad (2.54)$$

*Proof.* We observe that

$$\overline{D}_1 y_\ell = \frac{y_{\ell+1} - y_\ell}{\varepsilon} = y'(m_\ell) + O(\varepsilon^2). \quad (2.55)$$

Thus, if we use the Taylor expansion of  $\phi(2\overline{D}_1 y_\ell)$  around  $2y'(m_\ell)$ ,

$$\phi(2\overline{D}_1 y_\ell) = \phi(2y'(m_\ell)) + \phi'(\xi)[2\overline{D}_1 y_\ell - 2y'(m_\ell)], \quad (2.56)$$

where  $\xi$  is between  $2\overline{D}_1 y_\ell$  and  $2y'(m_\ell)$ . Hence,

$$\begin{aligned} |\phi(2\overline{D}_1 y_\ell) - \phi(2y'(m_\ell))| &\leq \max_{\xi} |\phi'(\xi)| |2\overline{D}_1 y_\ell - 2y'(m_\ell)| \\ &\leq c\varepsilon^2, \quad c \in \mathbb{R}. \end{aligned} \quad (2.57)$$

$\square$

Equation (2.36) will be examined in parts as follows

$$\begin{aligned}
A_{CB} - E_{\Omega_{a_1}, 2}^a \{y\} &= \varepsilon \sum_{K=(x_1, x_2)}^{(x_{N^*-2}, x_{N^*-1})} \phi(2y'(m_K)) - \varepsilon \sum_{\ell=1}^{N^*-2} \phi(\overline{D}_2 y_\ell) \\
&= \varepsilon \sum_{K=(x_1, x_2)}^{(x_{N^*-2}, x_{N^*-1})} \phi(2y'(m_K)) - \varepsilon \sum_{\ell=1}^{N^*-3} \phi(2y'(m_{\ell+1})) \\
&\quad - \frac{\varepsilon}{2} [\phi(\overline{D}_2 y_1) + \phi(\overline{D}_2 y_{N^*-2})] + O(\varepsilon^2) \\
&= \varepsilon \phi(2y'(m_{(x_1, x_2)})) + \varepsilon \phi(2y'(m_{(x_2, x_3)})) + \cdots \\
&\quad + \varepsilon \phi(2y'(m_{(x_{N^*-2}, x_{N^*-1})})) - \varepsilon \phi(2y'(m_2)) - \varepsilon \phi(2y'(m_3)) \cdots \\
&\quad - \varepsilon \phi(2y'(m_{N^*-2})) - \frac{\varepsilon}{2} [\phi(\overline{D}_2 y_1) + \phi(\overline{D}_2 y_{N^*-2})] + O(\varepsilon^2) \\
&= \varepsilon \phi(2y'(m_{(x_1, x_2)})) - \frac{\varepsilon}{2} [\phi(\overline{D}_2 y_1) + \phi(\overline{D}_2 y_{N^*-2})] + O(\varepsilon^2),
\end{aligned} \tag{2.58}$$

where Lemma 3 was applied. Then,

$$\begin{aligned}
B_{CB} - E_{\Gamma_1, 2}^D \{y\} &= \varepsilon \sum_{K=(x_{N^*-1}, x_{N^*})}^{(x_{N^*}, x_{N^*+1})} \phi(2y'(m_K)) - \frac{\varepsilon}{2} \phi(\overline{D}_2 y_{N^*-1}) \\
&\quad + \frac{1}{2} \phi' \left( \frac{y_{N^*+1} - y_{N^*-1}}{2\varepsilon} + \frac{y_{N^*+1} - y_{N^*}}{\varepsilon} \right) [y_{N^*-1} + y_{N^*+1} - 2y_{N^*}] \\
&= \varepsilon \phi(2y'(m_{(x_{N^*-1}, x_{N^*})})) + \varepsilon \phi(2y'(m_{(x_{N^*}, x_{N^*+1})})) - \frac{\varepsilon}{2} \phi(\overline{D}_2 y_{N^*-1}) \\
&\quad + \frac{1}{2} \phi' \left( \frac{y_{N^*+1} - y_{N^*-1}}{2\varepsilon} + \frac{y_{N^*+1} - y_{N^*}}{\varepsilon} \right) [y_{N^*-1} + y_{N^*+1} - 2y_{N^*}],
\end{aligned} \tag{2.59}$$

and

$$\begin{aligned}
\Gamma_{CB} - E_{\Omega_*, 2}^{a, CB} \{y\} &= \varepsilon \sum_{K=(x_{N^*+1}, x_{N^*+2})}^{(x_{N^{**}-2}, x_{N^{**}-1})} \phi(2y'(m_K)) - \varepsilon \sum_{\ell=N^*}^{N^{**}-1} \phi(2y'(m_\ell)) \\
&= \varepsilon \phi(2y'(m_{(x_{N^*+1}, x_{N^*+2})})) + \varepsilon \phi(2y'(m_{(x_{N^*+2}, x_{N^*+3})})) + \cdots \\
&\quad + \varepsilon \phi(2y'(m_{(x_{N^{**}-2}, x_{N^{**}-1})})) - \varepsilon \phi(2y'(m_{N^*})) \\
&\quad - \varepsilon \phi(2y'(m_{N^*+1})) - \cdots - \varepsilon \phi(2y'(m_{N^{**}-1})) + O(\varepsilon^2) \\
&= -\varepsilon \phi(2y'(m_{N^*})) - \varepsilon \phi(2y'(m_{N^{**}-1})) + O(\varepsilon^2),
\end{aligned} \tag{2.60}$$

where Lemma 5 was applied. Also,

$$\begin{aligned}
D_{CB} - E_{\Gamma_{2,2}}\{y\} &= \varepsilon \sum_{K=(x_{N^{**}-1}, x_{N^{**}})}^{(x_{N^{**}}, x_{N^{**}+1})} \phi(2y'(m_K)) - \frac{\varepsilon}{2} \phi(\overline{D}_2 y_{N^{**}-1}) \\
&\quad + \frac{1}{2} \phi' \left( \frac{y_{N^{**}} - y_{N^{**}-1}}{\varepsilon} + \frac{y_{N^{**}+1} - y_{N^{**}-1}}{2\varepsilon} \right) \\
&\quad [2y_{N^{**}} - y_{N^{**}-1} - y_{N^{**}+1}] \\
&= \varepsilon \phi(2y'(m_{(x_{N^{**}-1}, x_{N^{**}})})) + \varepsilon \phi(2y'(m_{(x_{N^{**}}, x_{N^{**}+1})})) - \frac{\varepsilon}{2} \phi(\overline{D}_2 y_{N^{**}-1}) \\
&\quad + \frac{1}{2} \phi' \left( \frac{y_{N^{**}} - y_{N^{**}-1}}{\varepsilon} + \frac{y_{N^{**}+1} - y_{N^{**}-1}}{2\varepsilon} \right) \\
&\quad [2y_{N^{**}} - y_{N^{**}-1} - y_{N^{**}+1}],
\end{aligned} \tag{2.61}$$

and finally

$$\begin{aligned}
G_{CB} - E_{\Omega_{a_2}, 2}^a\{y\} &= \varepsilon \sum_{K=(x_{N^{**}+1}, x_{N^{**}+2})}^{(x_N, x_{N+1})} \phi(2y'(m_K)) - \varepsilon \sum_{\ell=N^{**}}^N \phi(\overline{D}_2 y_\ell) \\
&= \varepsilon \sum_{K=(x_{N^{**}+1}, x_{N^{**}+2})}^{(x_N, x_{N+1})} \phi(2y'(m_K)) - \varepsilon \sum_{\ell=N^{**}}^{N-1} \phi(2y'(m_{\ell+1})) \quad (2.62) \\
&\quad - \frac{\varepsilon}{2} [\phi(\overline{D}_2 y_{N^{**}}) + \phi(\overline{D}_2 y_N)] + O(\varepsilon^2) \\
&= -\frac{\varepsilon}{2} [\phi(\overline{D}_2 y_{N^{**}}) + \phi(\overline{D}_2 y_N)] + O(\varepsilon^2),
\end{aligned}$$

where Lemma 4 was applied. Therefore, (2.36) becomes

$$\begin{aligned}
\Phi_2^{a,CB}(y) - \mathcal{E}_2^D\{y\} &= \varepsilon \phi(2y'(m_{(x_1, x_2)})) - \frac{\varepsilon}{2} [\phi(\overline{D}_2 y_1) + \phi(\overline{D}_2 y_{N^*-2})] \\
&\quad + \varepsilon \phi(2y'(m_{(x_{N^*-1}, x_{N^*})})) + \varepsilon \phi(2y'(m_{(x_{N^*}, x_{N^*+1})})) \\
&\quad - \frac{\varepsilon}{2} \phi(\overline{D}_2 y_{N^*-1}) + \frac{1}{2} \phi' \left( \frac{y_{N^*+1} - y_{N^*-1}}{2\varepsilon} + \frac{y_{N^*+1} - y_{N^*}}{\varepsilon} \right) \\
&\quad [y_{N^*-1} + y_{N^*+1} - 2y_{N^*}] - \varepsilon \phi(2y'(m_{N^*})) - \varepsilon \phi(2y'(m_{N^{**}-1})) \\
&\quad + \varepsilon \phi(2y'(m_{(x_{N^{**}-1}, x_{N^{**}})})) + \varepsilon \phi(2y'(m_{(x_{N^{**}}, x_{N^{**}+1})})) \\
&\quad - \frac{\varepsilon}{2} \phi(\overline{D}_2 y_{N^{**}-1}) + \frac{1}{2} \phi' \left( \frac{y_{N^{**}} - y_{N^{**}-1}}{\varepsilon} + \frac{y_{N^{**}+1} - y_{N^{**}-1}}{2\varepsilon} \right) \\
&\quad [2y_{N^{**}} - y_{N^{**}-1} - y_{N^{**}+1}] - \frac{\varepsilon}{2} [\phi(\overline{D}_2 y_{N^{**}}) + \phi(\overline{D}_2 y_N)] + O(\varepsilon^2) \\
&= \varepsilon \phi(2y'(m_{(x_1, x_2)})) - \frac{\varepsilon}{2} [\phi(\overline{D}_2 y_1) + \phi(\overline{D}_2 y_{N^*-2})] \\
&\quad + \varepsilon \phi(2y'(m_{(x_{N^*-1}, x_{N^*})})) - \frac{\varepsilon}{2} \phi(\overline{D}_2 y_{N^*-1}) \\
&\quad + \frac{1}{2} \phi' \left( \frac{y_{N^*+1} - y_{N^*-1}}{2\varepsilon} + \frac{y_{N^*+1} - y_{N^*}}{\varepsilon} \right) [y_{N^*-1} + y_{N^*+1} \\
&\quad - 2y_{N^*}] + \varepsilon \phi(2y'(m_{(x_{N^{**}}, x_{N^{**}+1})})) - \frac{\varepsilon}{2} \phi(\overline{D}_2 y_{N^{**}-1}) \\
&\quad + \frac{1}{2} \phi' \left( \frac{y_{N^{**}} - y_{N^{**}-1}}{\varepsilon} + \frac{y_{N^{**}+1} - y_{N^{**}-1}}{2\varepsilon} \right) [2y_{N^{**}} - y_{N^{**}-1} \\
&\quad - y_{N^{**}+1}] - \frac{\varepsilon}{2} [\phi(\overline{D}_2 y_{N^{**}}) + \phi(\overline{D}_2 y_N)] + O(\varepsilon^2).
\end{aligned} \tag{2.63}$$

Since  $m_\ell = m_{(x_\ell, x_{\ell+1})}$ , we conclude,

$$\begin{aligned}
\Phi_2^{a,CB}(y) - \mathcal{E}_2^D\{y\} &= \varepsilon \phi(2y'(m_1)) - \frac{\varepsilon}{2} [\phi(\overline{D}_2 y_1) + \phi(\overline{D}_2 y_{N^*-2})] \\
&\quad + \varepsilon \phi(2y'(m_{N^*-1})) - \frac{\varepsilon}{2} \phi(\overline{D}_2 y_{N^*-1}) \\
&\quad + \frac{1}{2} \phi' \left( \frac{y_{N^*+1} - y_{N^*-1}}{2\varepsilon} + \frac{y_{N^*+1} - y_{N^*}}{\varepsilon} \right) [y_{N^*-1} + y_{N^*+1} \\
&\quad - 2y_{N^*}] + \varepsilon \phi(2y'(m_{N^{**}})) - \frac{\varepsilon}{2} \phi(\overline{D}_2 y_{N^{**}-1}) \\
&\quad + \frac{1}{2} \phi' \left( \frac{y_{N^{**}} - y_{N^{**}-1}}{\varepsilon} + \frac{y_{N^{**}+1} - y_{N^{**}-1}}{2\varepsilon} \right) [2y_{N^{**}} - y_{N^{**}-1} \\
&\quad - y_{N^{**}+1}] - \frac{\varepsilon}{2} [\phi(\overline{D}_2 y_{N^{**}}) + \phi(\overline{D}_2 y_N)] + O(\varepsilon^2).
\end{aligned} \tag{2.64}$$

Notice that it remains to check what is the order of the boundary and interface terms. We will collect certain terms together and examine their order. Two lemmas will be displayed below so that they are applied to our final result right after.

**Lemma 6.** *For a smooth function  $y$  and a smooth function  $\phi$  whose derivatives are bounded we have*

$$\left| \phi' \left( \frac{y_{N^*+1} - y_{N^*-1}}{2\varepsilon} + \frac{y_{N^*+1} - y_{N^*}}{\varepsilon} \right) [y_{N^*-1} + y_{N^*+1} - 2y_{N^*}] \right| \leq O(\varepsilon^2). \tag{2.65}$$



*Proof.* Since  $\phi' \left( \frac{y_{N^*+1} - y_{N^*-1}}{2\varepsilon} + \frac{y_{N^*+1} - y_{N^*}}{\varepsilon} \right)$  is bounded (Assumption 2) we will only examine

$$[y_{N^*-1} + y_{N^*+1} - 2y_{N^*}]. \quad (2.66)$$

It is straightforward to check that

$$y_{N^*-1} + y_{N^*+1} - 2y_{N^*} = \varepsilon^2 y''(x_{N^*}) + O(\varepsilon^4). \quad (2.67)$$

Hence,

$$|\phi' \left( \frac{y_{N^*+1} - y_{N^*-1}}{2\varepsilon} + \frac{y_{N^*+1} - y_{N^*}}{\varepsilon} \right) [y_{N^*-1} + y_{N^*+1} - 2y_{N^*}]| \leq O(\varepsilon^2). \quad (2.68)$$

□

Similarly,

$$|\frac{1}{2}\phi' \left( \frac{y_{N^{**}} - y_{N^{**}-1}}{\varepsilon} + \frac{y_{N^{**}+1} - y_{N^{**}-1}}{2\varepsilon} \right) [2y_{N^{**}} - y_{N^{**}-1} - y_{N^{**}+1}]| \leq O(\varepsilon^2). \quad (2.69)$$

**Lemma 7.** *For a smooth function  $y$  and a smooth function  $\phi$  whose derivatives are bounded we have*

$$|\varepsilon\phi(2y'(m_{N^*-1})) - \frac{\varepsilon}{2}\phi(\overline{D}_2 y_{N^*-2}) - \frac{\varepsilon}{2}\phi(\overline{D}_2 y_{N^*-1})| \leq O(\varepsilon^2). \quad (2.70)$$

*Proof.* As before,

$$\begin{aligned} \overline{D}_2 y_{N^*-1} + \overline{D}_2 y_{N^*-2} &= 3y'(m_{N^*-1}) + y'(m_{N^*-1}) + O(\varepsilon^2) \\ &= 4y'(m_{N^*-1}) + O(\varepsilon^2), \end{aligned} \quad (2.71)$$

and so

$$\frac{1}{2}(\overline{D}_2 y_{N^*-1} + \overline{D}_2 y_{N^*-2}) = 2y'(m_{N^*-1}) + O(\varepsilon^2). \quad (2.72)$$

From (2.42) we obtain

$$\left| \frac{\phi(\overline{D}_2 y_{N^*-1}) + \phi(\overline{D}_2 y_{N^*-2})}{2} - \phi \left( \frac{\overline{D}_2 y_{N^*-1} + \overline{D}_2 y_{N^*-2}}{2} \right) \right| \leq c\varepsilon^2. \quad (2.73)$$

By expanding  $\phi \left( \frac{\overline{D}_2 y_{N^*-1} + \overline{D}_2 y_{N^*-2}}{2} \right)$  around  $2y'(m_{N^*-1})$  using Taylor expansion and Assumptions 1- 3 we obtain

$$\begin{aligned} \phi \left( \frac{\overline{D}_2 y_{N^*-1} + \overline{D}_2 y_{N^*-2}}{2} \right) &= \phi(2y'(m_{N^*-1})) \\ &\quad + \phi'(\xi) \left[ \frac{\overline{D}_2 y_{N^*-1} + \overline{D}_2 y_{N^*-2}}{2} - 2y'(m_{N^*-1}) \right], \end{aligned}$$

where  $\xi$  is between  $\left(\frac{\bar{D}_2 y_{N^*-1} + \bar{D}_2 y_{N^*-2}}{2}\right)$  and  $2y'(m_{N^*-1})$ . Therefore,

$$\begin{aligned} & \left| \phi\left(\frac{\bar{D}_2 y_{N^*-1} + \bar{D}_2 y_{N^*-2}}{2}\right) - \phi(2y'(m_{N^*-1})) \right| \\ & \leq \left| \phi'(\xi) \left[ \frac{\bar{D}_2 y_{N^*-1} + \bar{D}_2 y_{N^*-2}}{2} - 2y'(m_{N^*-1}) \right] \right| \\ & \leq \max_{\xi} |\phi'(\xi)| \left| \left[ \frac{\bar{D}_2 y_{N^*-1} + \bar{D}_2 y_{N^*-2}}{2} - 2y'(m_{N^*-1}) \right] \right| \\ & \leq c\varepsilon^2, \quad c \in \mathbb{R}. \end{aligned}$$

Hence, (2.70) holds.  $\square$

Similarly,

$$|\varepsilon\phi(2y'(m_{N^{**}})) - \frac{\varepsilon}{2}\phi(\bar{D}_2 y_{N^{**}-1}) - \frac{\varepsilon}{2}\phi(\bar{D}_2 y_{N^{**}})| \leq O(\varepsilon^2). \quad (2.74)$$

We are now ready to prove the main result of this section.

**Theorem 1.** *For a smooth function  $y$  the energy consistency error is of second order as follows*

$$|\Phi_2^{a,CB}(y) - \mathcal{E}_2^D\{y\}| \leq O(\varepsilon^2). \quad (2.75)$$

*Proof.* By applying Lemmas 6 and 7 and (2.69) and (2.74) to (2.64), the three remaining terms from (2.64) that need to be examined are

$$\varepsilon\phi(2y'(m_1)) - \frac{\varepsilon}{2}\phi(\bar{D}_2 y_1) - \frac{\varepsilon}{2}\phi(\bar{D}_2 y_N). \quad (2.76)$$

If we apply the periodicity condition,

$$y_{\ell+2+N} - y_{\ell+N} = y_{\ell+2} - y_{\ell}, \quad 1 \leq \ell \leq N, \quad (2.77)$$

to the last term of (2.76) we obtain

$$\phi(\bar{D}_2 y_N) = \phi(\bar{D}_2 y_0), \quad (2.78)$$

and (2.76) becomes

$$\varepsilon\phi(2y'(m_1)) - \frac{\varepsilon}{2}\phi(\bar{D}_2 y_1) - \frac{\varepsilon}{2}\phi(\bar{D}_2 y_0). \quad (2.79)$$

By following similar steps to Lemma 7 the following holds

$$|\varepsilon\phi(2y'(m_1)) - \frac{\varepsilon}{2}\phi(\bar{D}_2 y_1) - \frac{\varepsilon}{2}\phi(\bar{D}_2 y_0)| \leq O(\varepsilon^2). \quad (2.80)$$

Therefore,

$$|\Phi_2^{a,CB}(y) - \mathcal{E}_2^D\{y\}| \leq O(\varepsilon^2). \quad (2.81)$$

$\square$

## 2.4 Energy consistency for $\eta = 3$

### 2.4.1 Continuum Cauchy-Born potential energy for $\eta = 3$

Let

$$T = \{K \subset \Omega : K = (x_\ell, x_{\ell+1}), \quad \Omega = [x_1, x_{N+1}]\} \quad (2.82)$$

so

$$T = \{(x_1, x_2), (x_2, x_3), \dots, (x_N, x_{N+1})\}. \quad (2.83)$$

The continuum Cauchy-Born potential energy is

$$\Phi^{CB}(y) = \int_{\Omega} W_{CB}(y'(x)) dx = \sum_{K \in T} \int_K W_{CB}(y'(x)) dx, \quad (2.84)$$

where

$$W_{CB}(y'(x)) = \sum_{\eta} \phi(y'(x)\eta). \quad (2.85)$$

The atomistic Cauchy-Born energy is a second order approximation of the Cauchy-Born energy [21],

$$\Phi^{a,CB} = \varepsilon \sum_{K \in T} W_{CB}(y'(m_K)). \quad (2.86)$$

For  $\eta = 3$  this reduces to

$$\begin{aligned} \Phi_3^{CB}(y) = \varepsilon \sum_{K \in T} \phi(3y'(m_K)) = & \varepsilon [\phi(3y'(m_{(x_1, x_2)})) + \phi(3y'(m_{(x_2, x_3)})) + \dots \\ & + \phi(3y'(m_{(x_N, x_{N+1})}))]. \end{aligned} \quad (2.87)$$

### 2.4.2 Energy on the interfaces for $\eta = 3$

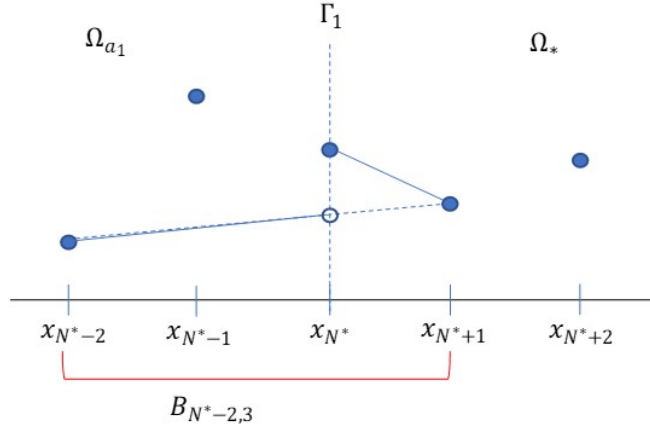
For the interfaces  $\Gamma_1 = x_{N^*}$  and  $\Gamma_2 = x_{N^{**}}$  we need to consider bonds  $B_{\ell,3} = [x_\ell, x_{\ell+3}]$  intersecting  $\Gamma_1$  or  $\Gamma_2$ . There are two bonds that intersect interface  $\Gamma_1$ ,  $B_{N^*-2,3}$  and  $B_{N^*-1,3}$  and two bonds that intersect interface  $\Gamma_2$ ,  $B_{N^{**}-2,3}$  and  $B_{N^{**}-1,3}$ , Figure 2.9. Let  $y^{\ell,3}$  be the continuous, piecewise linear function on  $B_{\ell,3}$ , such that for  $\Gamma_1$ ,  $y^{\ell,3}$  is linear on  $(x_\ell, x_{N^*})$  and linear on each  $I_\ell$  of  $(x_{N^*}, x_{\ell+3})$ , where  $I_\ell = (x_\ell, x_{\ell+1})$ , Figures 2.5 and 2.6. For  $\Gamma_2$ ,  $y^{\ell,3}$  is linear on each  $I_\ell$  of  $(x_\ell, x_{N^{**}})$  and linear for  $(x_{N^{**}}, x_{\ell+3})$ , Figures 2.7 and 2.8. For  $\Gamma_1$ , let  $y^{\ell,3-}$  and  $y^{\ell,3+}$  be the limits taken from  $\Omega_a$  and  $\Omega_*$  respectively as follows

$$y^{\ell,3+}(x_{N^*}) = y_{N^*}, \quad (2.88)$$

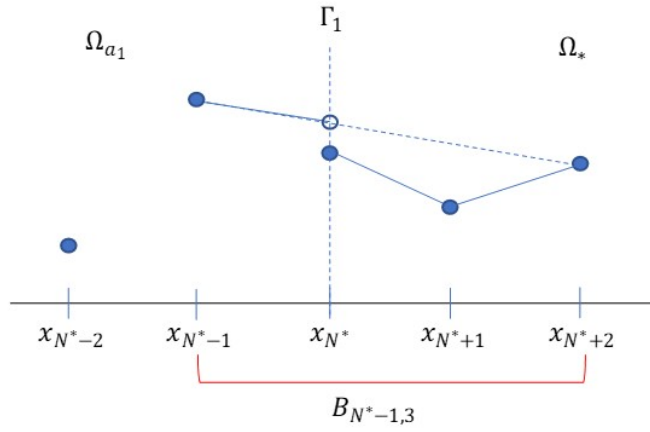
$$y^{\ell,3-}(x_{N^*}) = y_\ell + \left( \frac{y_{\ell+3} - y_\ell}{x_{\ell+3} - x_\ell} \right) (x_{N^*} - x_\ell). \quad (2.89)$$

Their corresponding derivatives are

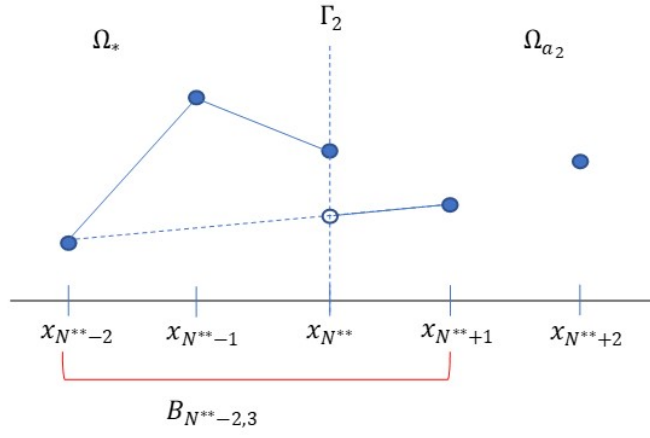
$$(y^{\ell,3})'^+(x_{N^*}) = \frac{y_{N^*+1} - y_{N^*}}{\varepsilon}, \quad (2.90)$$



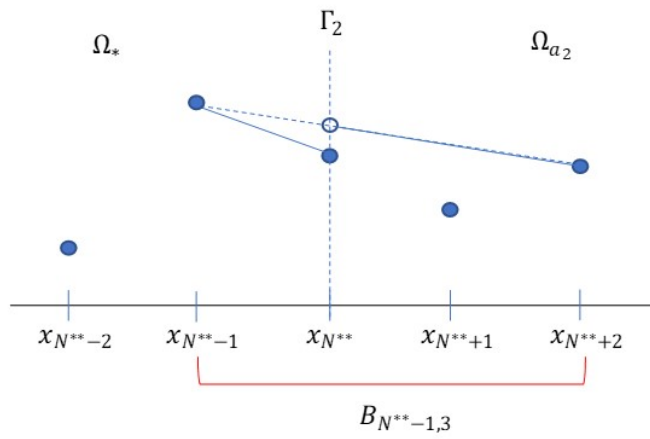
**Figure 2.5:** An example of  $y^{N^*-2,3}$  on the bond  $B_{N^*-2,3}$  that intersects interface  $\Gamma_1$ .



**Figure 2.6:** An example of  $y^{N^*-1,3}$  on the bond  $B_{N^*-1,3}$  that intersects interface  $\Gamma_1$ .



**Figure 2.7:** An example of  $y^{N^{**}-2,3}$  on the bond  $B_{N^{**}-2,3}$  that intersects interface  $\Gamma_2$ , ( $\eta_\Gamma = 2$ ).



**Figure 2.8:** An example of  $y^{N^{**}-1,3}$  on the bond  $B_{N^{**}-1,3}$  that intersects interface  $\Gamma_2$ , ( $\eta_\Gamma = 1$ ).

$$(y^{\ell,3})'^-(x_{N^*}) = \frac{y_{\ell+3} - y_\ell}{x_{\ell+3} - x_\ell}. \quad (2.91)$$

For  $\Gamma_2$ , let  $y^{\ell,3-}$  and  $y^{\ell,3+}$  be the limits taken from  $\Omega_*$  and  $\Omega_a$  respectively

$$y^{\ell,3+}(x_{N^{**}}) = y_\ell + \left( \frac{y_{\ell+3} - y_\ell}{x_{\ell+3} - x_\ell} \right) (x_{N^{**}} - x_\ell), \quad (2.92)$$

$$y^{\ell,3-}(x_{N^{**}}) = y_{N^{**}}. \quad (2.93)$$

Their corresponding derivatives are

$$(y^{\ell,3})'^+(x_{N^{**}}) = \frac{y_{\ell+3} - y_\ell}{x_{\ell+3} - x_\ell}, \quad (2.94)$$

$$(y^{\ell,3})'^-(x_{N^{**}}) = \frac{y_{N^{**}} - y_{N^{**}-1}}{\varepsilon}. \quad (2.95)$$

The form of the energy is the same for both interfaces  $\Gamma_1$  and  $\Gamma_2$  and so for simplicity we will define the energy for a general  $\Gamma$ , (1.40). To compute the energy due to bonds intersecting the interface, first notice that

$$\begin{aligned} \sum_{\substack{\ell \in \mathcal{L} \\ B_{\ell,3} \cap \Gamma \neq \emptyset}} \frac{1}{3} \int_{B_{\ell,3}} \chi_{\Omega_a} \phi(3(y^{\ell,3})') dx &= \sum_{\substack{\ell \in \mathcal{L} \\ B_{\ell,3} \cap \Gamma \neq \emptyset}} |\Omega_a \cap B_{\ell,3}| \frac{1}{3} \phi \left( 3 \frac{y_{\ell+3} - y_\ell}{3\varepsilon} \right) \\ &= \sum_{\substack{\ell \in \mathcal{L} \\ B_{\ell,3} \cap \Gamma \neq \emptyset}} \frac{1}{3} |\Omega_a \cap B_{\ell,3}| \phi(\bar{D}_3 y_\ell), \end{aligned} \quad (2.96)$$

where  $|\Omega_a \cap B_{\ell,3}|$  is the size of the intersection of the atomistic region  $\Omega_a$  and the bond  $B_{\ell,3}$ . Then, taking into account the terms of discontinuous coupling across the interface  $\Gamma$ , the energy due to bonds intersecting the interface, (1.40), is

$$\begin{aligned} E_{\Gamma,3}^D\{y\} &= \sum_{\substack{\ell \in \mathcal{L} \\ B_{\ell,3} \cap \Gamma \neq \emptyset}} \frac{1}{3} \left[ \int_{B_{\ell,3}} \chi_{\Omega_a} \phi(3(y^{\ell,3})') dx - \int_{B_{\ell,3} \cap \Gamma} \phi'(\{3(y^{\ell,3})'\}) \cdot \llbracket 3y^{\ell,3} \rrbracket dS \right] \\ &= \frac{1}{3} \left[ \sum_{\substack{\ell \in \mathcal{L} \\ B_{\ell,3} \cap \Gamma \neq \emptyset}} |\Omega_a \cap B_{\ell,3}| \phi(\bar{D}_3 y_\ell) - \phi'(\{3(y^{\ell,3})'\}) \llbracket 3y^{\ell,3} \rrbracket \right] \\ &= \frac{1}{3} \left[ \sum_{\substack{\ell \in \mathcal{L} \\ B_{\ell,3} \cap \Gamma \neq \emptyset}} |\Omega_a \cap B_{\ell,3}| \phi(\bar{D}_3 y_\ell) \right. \\ &\quad \left. - \phi' \left( \frac{1}{2} \{3(y^{\ell,3})'^- + 3(y^{\ell,3})'^+\} \right) [3(y^{\ell,3})^- - 3(y^{\ell,3})^+] \right]. \end{aligned} \quad (2.97)$$

The bonds  $B_{\ell,3}$  that intersect the interface  $\Gamma_1$  are  $B_{N^*-2,3}$  and  $B_{N^*-1,3}$  and hence

$$\begin{aligned}
E_{\Gamma_1,3}^D\{y\} &= \frac{2\varepsilon}{3}\phi(\overline{D}_3 y_{N^*-2}) + \frac{\varepsilon}{3}\phi(\overline{D}_3 y_{N^*-1}) \\
&\quad - \frac{1}{3}\phi'(\{ \{ (y^{N^*-2,3})'^- + (y^{N^*-2,3})'^+ \} \}) [3(y^{N^*-2,3})^- - 3(y^{N^*-2,3})^+] \\
&\quad - \frac{1}{3}\phi'(\{ \{ (y^{N^*-1,3})'^- + (y^{N^*-1,3})'^+ \} \}) [3(y^{N^*-1,3})^- - 3(y^{N^*-1,3})^+] \\
&= \frac{2\varepsilon}{3}\phi(\overline{D}_3 y_{N^*-2}) - \frac{1}{3}\phi' \left( \frac{3}{2} \left\{ \frac{y_{N^*+1} - y_{N^*-2}}{x_{N^*+1} - x_{N^*-2}} + \frac{y_{N^*+1} - y_{N^*}}{\varepsilon} \right\} \right) [3y_{N^*-2} \\
&\quad + 3 \left( \frac{y_{N^*+1} - y_{N^*-2}}{x_{N^*+1} - x_{N^*-2}} \right) (x_{N^*} - x_{N^*-2}) - 3y_{N^*}] \\
&\quad + \frac{\varepsilon}{3}\phi(\overline{D}_3 y_{N^*-1}) - \frac{1}{3}\phi' \left( \frac{3}{2} \left\{ \frac{y_{N^*+2} - y_{N^*-1}}{x_{N^*+2} - x_{N^*-1}} + \frac{y_{N^*+1} - y_{N^*}}{\varepsilon} \right\} \right) [3y_{N^*-1} \\
&\quad + 3 \left( \frac{y_{N^*+2} - y_{N^*-1}}{x_{N^*+2} - x_{N^*-1}} \right) (x_{N^*} - x_{N^*-1}) - 3y_{N^*}] \\
&= \frac{2\varepsilon}{3}\phi(\overline{D}_3 y_{N^*-2}) - \frac{1}{3}\phi' \left( \frac{3}{2} \left\{ \frac{y_{N^*+1} - y_{N^*-2}}{3\varepsilon} + \frac{y_{N^*+1} - y_{N^*}}{\varepsilon} \right\} \right) [y_{N^*-2} \\
&\quad + 2y_{N^*+1} - 3y_{N^*}] + \frac{\varepsilon}{3}\phi(\overline{D}_3 y_{N^*-1}) \\
&\quad - \frac{1}{3}\phi' \left( \frac{3}{2} \left\{ \frac{y_{N^*+2} - y_{N^*-1}}{3\varepsilon} + \frac{y_{N^*+1} - y_{N^*}}{\varepsilon} \right\} \right) [2y_{N^*-1} + y_{N^*+2} \\
&\quad - 3y_{N^*}].
\end{aligned} \tag{2.98}$$

Similarly, the bonds  $B_{\ell,3}$  that intersect the interface  $\Gamma_2$  are  $B_{N^{**}-2,2}$  and  $B_{N^{**}-1,3}$

and hence,

$$\begin{aligned}
E_{\Gamma_2,3}^D\{y\} &= \frac{2\varepsilon}{3}\phi(\overline{D}_3 y_{N^{**}-2}) + \frac{\varepsilon}{3}\phi(\overline{D}_3 y_{N^{**}-1}) \\
&\quad - \frac{1}{3}\phi'(\{\{(y^{N^{**}-2,3})'^- + (y^{N^{**}-2,3})'^+\}\})[3(y^{N^{**}-2,3})^- - 3(y^{N^{**}-2,3})^+] \\
&\quad - \frac{1}{3}\phi'(\{\{(y^{N^{**}-1,3})'^- + (y^{N^{**}-1,3})'^+\}\})[3(y^{N^{**}-1,3})^- - 3(y^{N^{**}-1,3})^+] \\
&= \frac{2\varepsilon}{3}\phi(\overline{D}_3 y_{N^{**}-2}) - \frac{1}{3}\phi'\left(\frac{3}{2}\left\{\frac{y_{N^{**}} - y_{N^{**}-1}}{\varepsilon} + \frac{y_{N^{**}+1} - y_{N^{**}-2}}{x_{N^{**}+1} - x_{N^{**}-2}}\right\}\right)[3y_{N^{**}} \\
&\quad - 3y_{N^{**}-2} - 3\left(\frac{y_{N^{**}+1} - y_{N^{**}-2}}{x_{N^{**}+1} - x_{N^{**}-2}}\right)(x_{N^{**}} - x_{N^{**}-2})] \\
&\quad + \frac{\varepsilon}{3}\phi(\overline{D}_3 y_{N^{**}-1}) - \frac{1}{3}\phi'\left(\frac{3}{2}\left\{\frac{y_{N^{**}} - y_{N^{**}-1}}{\varepsilon} + \frac{y_{N^{**}+2} - y_{N^{**}-1}}{x_{N^{**}+2} - x_{N^{**}-1}}\right\}\right)[3y_{N^{**}} \\
&\quad - 3y_{N^{**}-1} - 3\left(\frac{y_{N^{**}+2} - y_{N^{**}-1}}{x_{N^{**}+2} - x_{N^{**}-1}}\right)(x_{N^{**}} - x_{N^{**}-1})] \\
&= \frac{2\varepsilon}{3}\phi(\overline{D}_3 y_{N^{**}-2}) + \frac{\varepsilon}{3}\phi(\overline{D}_3 y_{N^{**}-1}) \\
&\quad - \frac{1}{3}\phi'\left(\frac{3}{2}\left\{\frac{y_{N^{**}} - y_{N^{**}-1}}{\varepsilon} + \frac{y_{N^{**}+1} - y_{N^{**}-2}}{3\varepsilon}\right\}\right)[3y_{N^{**}} - y_{N^{**}-2} \\
&\quad - 2y_{N^{**}+1}] - \frac{1}{3}\phi'\left(\frac{3}{2}\left\{\frac{y_{N^{**}} - y_{N^{**}-1}}{\varepsilon} + \frac{y_{N^{**}+2} - y_{N^{**}-1}}{3\varepsilon}\right\}\right)[3y_{N^{**}} \\
&\quad - 2y_{N^{**}-1} - y_{N^{**}+2}].
\end{aligned} \tag{2.99}$$

### 2.4.3 Atomistic to Continuum Coupled Energy for $\eta = 3$

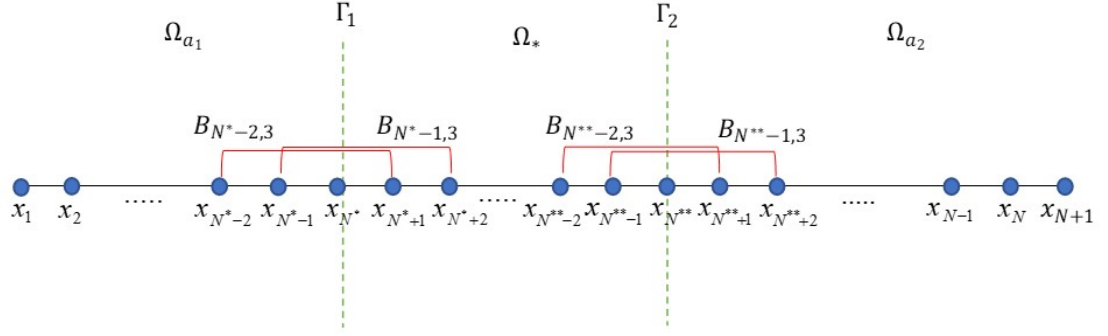
Recall that the total coupling energy is:

$$\mathcal{E}_{bv}^D\{y\} = \sum_{\eta \in R} \mathcal{E}_{\eta}^D\{y\}, \tag{2.100}$$

where

$$\mathcal{E}_{\eta}^D\{y\} = E_{\Omega_{a_1},\eta}^a\{y\} + E_{\Gamma_1,\eta}^D\{y\} + E_{\Omega_{*},\eta}^{a,CB}\{y\} + E_{\Gamma_2,\eta}^D\{y\} + E_{\Omega_{a_2},\eta}^a\{y\}. \tag{2.101}$$



**Figure 2.9:** The atomistic to continuum coupling domain

For fixed  $\eta = 3$ ,

$$\begin{aligned}
E_{\Omega_{a_1},3}^a \{y\} &= \varepsilon \sum_{\ell=1}^{N^*-3} \phi(\bar{D}_3 y_\ell) \\
E_{\Gamma_1,3}^D \{y\} &= \frac{2\varepsilon}{3} \phi(\bar{D}_3 y_{N^*-2}) + \frac{\varepsilon}{3} \phi(\bar{D}_3 y_{N^*-1}) \\
&\quad - \frac{1}{3} \phi' \left( \frac{3}{2} \left\{ \frac{y_{N^*+1} - y_{N^*-2}}{3\varepsilon} + \frac{y_{N^*+1} - y_{N^*}}{\varepsilon} \right\} \right) [y_{N^*-2} + 2y_{N^*+1} - 3y_{N^*}] \\
&\quad - \frac{1}{3} \phi' \left( \frac{3}{2} \left\{ \frac{y_{N^*+2} - y_{N^*-1}}{3\varepsilon} + \frac{y_{N^*+1} - y_{N^*}}{\varepsilon} \right\} \right) [2y_{N^*-1} + y_{N^*+2} - 3y_{N^*}] \\
E_{\Omega_*,3}^{a,CB} \{y\} &= \varepsilon \sum_{\ell=N^*}^{N^{**}-1} \phi(3\bar{D}_1 y_\ell) \\
E_{\Gamma_2,3}^D \{y\} &= \frac{2\varepsilon}{3} \phi(\bar{D}_3 y_{N^{**}-2}) + \frac{\varepsilon}{3} \phi(\bar{D}_3 y_{N^{**}-1}) \\
&\quad - \frac{1}{3} \phi' \left( \frac{3}{2} \left\{ \frac{y_{N^{**}} - y_{N^{**}-1}}{\varepsilon} + \frac{y_{N^{**}+1} - y_{N^{**}-2}}{3\varepsilon} \right\} \right) [3y_{N^{**}} - y_{N^{**}-2} \\
&\quad - 2y_{N^{**}+1}] - \frac{1}{3} \phi' \left( \frac{3}{2} \left\{ \frac{y_{N^{**}} - y_{N^{**}-1}}{\varepsilon} + \frac{y_{N^{**}+2} - y_{N^{**}-1}}{3\varepsilon} \right\} \right) [3y_{N^{**}} \\
&\quad - 2y_{N^{**}-1} - y_{N^{**}+2}] \\
E_{\Omega_{a_2},3}^a \{y\} &= \varepsilon \sum_{\ell=N^{**}}^N \phi(\bar{D}_3 y_\ell).
\end{aligned} \tag{2.102}$$

## 2.5 Comparison of coupled energy with continuum energy for $\eta = 3$

We split the continuum energy to correspond to the domains of (2.102), as follows

$$\begin{aligned}
\Phi_3^{a,CB}(y) = & \varepsilon \sum_{K=(x_1,x_2)}^{(x_{N^*-3},x_{N^*-2})} \phi(3y'(m_K)) + \varepsilon \sum_{K=(x_{N^*-2},x_{N^*-1})}^{(x_{N^*},x_{N^*+1})} \phi(3y'(m_K)) \\
& + \varepsilon \sum_{K=(x_{N^*+1},x_{N^*+2})}^{(x_{N^{**}-2},x_{N^{**}-1})} \phi(3y'(m_K)) + \varepsilon \sum_{K=(x_{N^{**}-1},x_{N^{**}})}^{(x_{N^{**}},x_{N^{**}+1})} \phi(3y'(m_K)) \\
& + \varepsilon \sum_{K=(x_{N^{**}+1},x_{N^{**}+2})}^{(x_N,x_{N+1})} \phi(3y'(m_K)) \\
= & A_{CB} + B_{CB} + \Gamma_{CB} + D_{CB} + G_{CB}.
\end{aligned} \tag{2.103}$$

We will compute  $\Phi_3^{a,CB}(y) - \mathcal{E}_3^D\{y\}$  as follows

$$\begin{aligned}
\Phi_3^{CB}(y) - \mathcal{E}_2^D\{y\} = & A_{CB} - E_{\Omega_{a_1},3}^a\{y\} + B_{CB} - E_{\Gamma_{1,3}}^D\{y\} + \Gamma_{CB} - E_{\Omega_{*,3}}^{a,CB}\{y\} \\
& + D_{CB} - E_{\Gamma_{2,3}}^D\{y\} + G_{CB} - E_{\Omega_{a_2},3}^a\{y\} \\
= & \varepsilon \sum_{K=(x_1,x_2)}^{(x_{N^*-3},x_{N^*-2})} \phi(3y'(m_K)) - \varepsilon \sum_{\ell=1}^{N^*-3} \phi(\bar{D}_3 y_\ell) \\
& + \varepsilon \sum_{K=(x_{N^*-2},x_{N^*-1})}^{(x_{N^*},x_{N^*+1})} \phi(3y'(m_K)) - \frac{2\varepsilon}{3} \phi(\bar{D}_3 y_{N^*-2}) - \frac{\varepsilon}{3} \phi(\bar{D}_3 y_{N^*-1}) \\
& + \frac{1}{3} \phi' \left( \frac{3}{2} \left\{ \frac{y_{N^*+1} - y_{N^*-2}}{x_{N^*+1} - x_{N^*-2}} + \frac{y_{N^*+1} - y_{N^*}}{\varepsilon} \right\} \right) [y_{N^*-2} + 2y_{N^*+1} \\
& - 3y_{N^*}] + \frac{1}{3} \phi' \left( \frac{3}{2} \left\{ \frac{y_{N^*+2} - y_{N^*-1}}{x_{N^*+2} - x_{N^*-1}} + \frac{y_{N^*+1} - y_{N^*}}{2\varepsilon} \right\} \right) [2y_{N^*-1} \\
& + y_{N^*+2} - 3y_{N^*}] + \varepsilon \sum_{K=(x_{N^*+1},x_{N^*+2})}^{(x_{N^{**}-2},x_{N^{**}-1})} \phi(3y'(m_K)) \\
& - \varepsilon \sum_{\ell=N^*}^{N^{**}-1} \phi(3\bar{D}_1 y_\ell) + \varepsilon \sum_{K=(x_{N^{**}-1},x_{N^{**}})}^{(x_{N^{**}},x_{N^{**}+1})} \phi(3y'(m_K)) \\
& - \frac{2\varepsilon}{3} \phi(\bar{D}_3 y_{N^{**}-2}) - \frac{\varepsilon}{3} \phi(\bar{D}_3 y_{N^{**}-1}) \\
& + \frac{1}{3} \phi' \left( \frac{3}{2} \left\{ \frac{y_{N^{**}} - y_{N^{**}-1}}{2\varepsilon} + \frac{y_{N^{**}+1} - y_{N^{**}-2}}{3\varepsilon} \right\} \right) [3y_{N^{**}} - y_{N^{**}-2} \\
& - 2y_{N^{**}+1}] + \frac{1}{3} \phi' \left( \frac{3}{2} \left\{ \frac{y_{N^{**}} - y_{N^{**}-1}}{\varepsilon} + \frac{y_{N^{**}+2} - y_{N^{**}-1}}{3\varepsilon} \right\} \right)
\end{aligned}$$

$$\begin{aligned}
& [3y_{N^{**}} - 2y_{N^{**}-1} - y_{N^{**}+2}] + \varepsilon \sum_{K=(x_{N^{**}+1}, x_{N^{**}+2})}^{(x_N, x_{N+1})} \phi(3y'(m_K)) \\
& - \varepsilon \sum_{\ell=N^{**}}^N \phi(\bar{D}_3 y_\ell).
\end{aligned} \tag{2.104}$$

As in the case of  $\eta = 2$ , the three lemmas below will be applied to 2.104.

**Lemma 8.** *For a smooth function  $y$  and a smooth function  $\phi$  whose derivatives are bounded we have*

$$\begin{aligned}
E_{\Omega_{a_1}, 3}^a \{y\} &= \varepsilon \sum_{\ell=1}^{N^*-3} \phi(\bar{D}_3 y_\ell) \\
&= \varepsilon \sum_{\ell=1}^{N^*-5} \phi(2y'(m_{\ell+2})) + \frac{\varepsilon}{3} [2\phi(\bar{D}_3 y_1) + \phi(\bar{D}_3 y_2)] \\
&\quad + \frac{\varepsilon}{3} [2\phi(\bar{D}_3 y_{N^*-3}) + \phi(\bar{D}_3 y_{N^*-4})] + O(\varepsilon^2).
\end{aligned} \tag{2.105}$$

*Proof.* We will start by looking at  $E_{\Omega_{a_1}, 3}^a \{y\}$  and we will introduce the following symmetry splitting

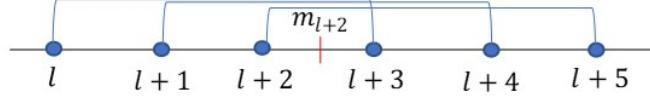
$$\begin{aligned}
E_{\Omega_{a_1}, 3}^a \{y\} &= \varepsilon \sum_{\ell=1}^{N^*-3} \phi(\bar{D}_3 y_\ell) \\
&= \frac{\varepsilon}{3} \left\{ [2\phi(\bar{D}_3 y_1) + \phi(\bar{D}_3 y_2)] + [\phi(\bar{D}_3 y_1) + \phi(\bar{D}_3 y_2) + \phi(\bar{D}_3 y_3)] \right. \\
&\quad + [\phi(\bar{D}_3 y_2) + \phi(\bar{D}_3 y_3) + \phi(\bar{D}_3 y_4)] + \cdots + [\phi(\bar{D}_3 y_{N^*-5}) + \phi(\bar{D}_3 y_{N^*-4}) \\
&\quad \left. + \phi(\bar{D}_3 y_{N^*-3})] + [2\phi(\bar{D}_3 y_{N^*-3}) + \phi(\bar{D}_3 y_{N^*-4})] \right\}.
\end{aligned} \tag{2.106}$$

Therefore,

$$\begin{aligned}
\varepsilon \sum_{\ell=1}^{N^*-3} \phi(\bar{D}_3 y_\ell) &= \varepsilon \sum_{\ell=1}^{N^*-3} \frac{1}{3} [\phi(\bar{D}_3 y_\ell) + \phi(\bar{D}_3 y_{\ell+1}) + \phi(\bar{D}_3 y_{\ell+2})] \\
&\quad + \frac{\varepsilon}{3} [2\phi(\bar{D}_3 y_1) + \phi(\bar{D}_3 y_2)] + \frac{\varepsilon}{3} [2\phi(\bar{D}_3 y_{N^*-3}) + \phi(\bar{D}_3 y_{N^*-4})].
\end{aligned} \tag{2.107}$$

Let  $m_{\ell+2}$  denote the middle point between  $x_{\ell+2}$  and  $x_{\ell+3}$ , Figure 2.10. Observe,

$$\begin{aligned}
\bar{D}_3 y_\ell + \bar{D}_3 y_{\ell+1} + \bar{D}_3 y_{\ell+2} &= \frac{y_{\ell+3} - y_\ell}{\varepsilon} + \frac{y_{\ell+4} - y_{\ell+1}}{\varepsilon} + \frac{y_{\ell+5} - y_{\ell+2}}{\varepsilon} \\
&= \frac{y_{\ell+5} - y_\ell}{\varepsilon} + \frac{y_{\ell+4} - y_{\ell+1}}{\varepsilon} + \frac{y_{\ell+3} - y_{\ell+2}}{\varepsilon} \\
&= 5y'(m_{\ell+2}) + 3y'(m_{\ell+2}) + y'(m_{\ell+2}) + O(\varepsilon^2) \\
&= 9y'(m_{\ell+2}) + O(\varepsilon^2).
\end{aligned} \tag{2.108}$$

**Figure 2.10:** Displaying  $m_{\ell+2}$ 

Hence,

$$\frac{1}{3}(\overline{D}_3 y_\ell + \overline{D}_3 y_{\ell+1} + \overline{D}_3 y_{\ell+2}) = 3y'(m_{\ell+2}) + O(\varepsilon^2). \quad (2.109)$$

Since we have assumed that  $\phi$  is smooth (Assumption 1) and that its derivatives are bounded (Assumption 3) we can expand  $\phi(a)$ ,  $\phi(b)$  and  $\phi(c)$  using Taylor expansion, around  $\left(\frac{a+b+c}{3}\right)$  and we obtain

$$\begin{aligned} \phi(a) &= \phi\left(\frac{a+b+c}{3}\right) - \phi'\left(\frac{a+b+c}{3}\right)\left(\frac{2a-b-c}{3}\right) + \frac{1}{2}\phi''(\xi_1)\left(\frac{2a-b-c}{3}\right)^2, \\ \phi(b) &= \phi\left(\frac{a+b+c}{3}\right) + \phi'\left(\frac{a+b+c}{3}\right)\left(\frac{2b-a-c}{3}\right) + \frac{1}{2}\phi''(\xi_2)\left(\frac{2b-a-c}{3}\right)^2, \\ \phi(c) &= \phi\left(\frac{a+b+c}{3}\right) + \phi'\left(\frac{a+b+c}{3}\right)\left(\frac{2c-b-a}{3}\right) + \frac{1}{2}\phi''(\xi_3)\left(\frac{2c-b-a}{3}\right)^2, \end{aligned}$$

where  $\xi_1 \in \left(a, \frac{a+b+c}{3}\right)$ ,  $\xi_2$  is between  $\frac{a+b+c}{3}$  and  $b$  and  $\xi_3 \in \left(\frac{a+b+c}{3}, c\right)$ . Adding  $\phi(a)$ ,  $\phi(b)$  and  $\phi(c)$  and after expanding the second order terms and collecting the terms we obtain the following condition

$$\left| \frac{\phi(a) + \phi(b) + \phi(c)}{3} - \phi\left(\frac{a+b+c}{3}\right) \right| \leq C(|a-b|^2 + |b-c|^2 + |c-a|^2), \quad C \in \mathbb{R}. \quad (2.110)$$

By applying the above condition we yield

$$\left| \frac{\phi(\overline{D}_3 y_\ell) + \phi(\overline{D}_3 y_{\ell+1}) + \phi(\overline{D}_3 y_{\ell+2})}{3} - \phi\left(\frac{\overline{D}_3 y_\ell + \overline{D}_3 y_{\ell+1} + \overline{D}_3 y_{\ell+2}}{3}\right) \right| \leq C\varepsilon^2. \quad (2.111)$$

In addition,

$$\begin{aligned} \phi\left(\frac{\overline{D}_3 y_\ell + \overline{D}_3 y_{\ell+1} + \overline{D}_3 y_{\ell+2}}{3}\right) &= \\ \phi(3y'(m_{\ell+2})) + \phi'(\xi) \left[ \frac{\overline{D}_3 y_\ell + \overline{D}_3 y_{\ell+1} + \overline{D}_3 y_{\ell+2}}{3} - 3y'(m_{\ell+2}) \right], \end{aligned} \quad (2.112)$$

where  $\xi$  is between  $\left(\frac{\overline{D}_3 y_\ell + \overline{D}_3 y_{\ell+1} + \overline{D}_3 y_{\ell+2}}{3}\right)$  and  $3y'(m_{\ell+2})$ .

Hence,

$$\begin{aligned}
& \left| \phi\left(\frac{\bar{D}_3 y_\ell + \bar{D}_3 y_{\ell+1} + \bar{D}_3 y_{\ell+2}}{3}\right) - \phi(3y'(m_{\ell+2})) \right| \\
& \leq \left| \phi'(\xi) \left[ \frac{\bar{D}_3 y_\ell + \bar{D}_3 y_{\ell+1} + \bar{D}_3 y_{\ell+2}}{3} - 3y'(m_{\ell+2}) \right] \right| \\
& \leq \max_{\xi} |\phi'(\xi)| \left| \left[ \frac{\bar{D}_3 y_\ell + \bar{D}_3 y_{\ell+1} + \bar{D}_3 y_{\ell+2}}{3} - 3y'(m_{\ell+2}) \right] \right| \\
& \leq c\varepsilon^2, \quad c \in \mathbb{R}.
\end{aligned} \tag{2.113}$$

due to Assumption 3. Therefore,

$$\begin{aligned}
E_{\Omega_{a_1},3}^a\{y\} &= \varepsilon \sum_{\ell=1}^{N^*-3} \phi(\bar{D}_3 y_\ell) = \varepsilon \sum_{\ell=1}^{N^*-5} \phi(3y'(m_{\ell+2})) + \frac{\varepsilon}{3} [2\phi(\bar{D}_3 y_1) + \phi(\bar{D}_3 y_2)] \\
&\quad + \frac{\varepsilon}{3} [2\phi(\bar{D}_3 y_{N^*-3}) + \phi(\bar{D}_3 y_{N^*-4})] + O(\varepsilon^2).
\end{aligned} \tag{2.114}$$

□

**Lemma 9.** *For a smooth function  $y$  and a smooth function  $\phi$  we have*

$$\begin{aligned}
E_{\Omega_{a_2},3}^a\{y\} &= \varepsilon \sum_{\ell=N^{**}}^N \phi(\bar{D}_3 y_\ell) \\
&= \varepsilon \sum_{\ell=N^{**}}^N \phi(3y'(m_{\ell+2})) + \frac{\varepsilon}{3} [2\phi(\bar{D}_3 y_{N^{**}}) + \phi(\bar{D}_3 y_{N^{**}+1})] \\
&\quad + \frac{\varepsilon}{3} [2\phi(\bar{D}_3 y_N) + \phi(\bar{D}_3 y_{N-1})] + O(\varepsilon^2).
\end{aligned} \tag{2.115}$$

*Proof.* We will start by looking at  $E_{\Omega_{a_2},3}^a\{y\}$  and we will introduce the following symmetry splitting

$$\begin{aligned}
E_{\Omega_{a_2},3}^a\{y\} &= \varepsilon \sum_{\ell=N^{**}}^N \phi(\bar{D}_3 y_\ell) \\
&= \frac{\varepsilon}{3} \left\{ [2\phi(\bar{D}_3 y_{N^{**}}) + \phi(\bar{D}_3 y_{N^{**}+1})] + [\phi(\bar{D}_3 y_{N^{**}}) + \phi(\bar{D}_3 y_{N^{**}+1}) \right. \\
&\quad + \phi(\bar{D}_3 y_{N^{**}+2})] + [\phi(\bar{D}_3 y_{N^{**}+1}) + \phi(\bar{D}_3 y_{N^{**}+2}) + \phi(\bar{D}_3 y_{N^{**}+3})] + \cdots \\
&\quad \left. + [\phi(\bar{D}_3 y_{N-2}) + \phi(\bar{D}_3 y_{N-1}) + \phi(\bar{D}_3 y_N)] + [2\phi(\bar{D}_3 y_N) + \phi(\bar{D}_3 y_{N-1})] \right\}.
\end{aligned} \tag{2.116}$$

Therefore,

$$\begin{aligned}
\varepsilon \sum_{\ell=N^{**}}^N \phi(\bar{D}_3 y_\ell) &= \varepsilon \sum_{\ell=N^{**}}^{N-2} \frac{1}{3} [\phi(\bar{D}_3 y_\ell) + \phi(\bar{D}_3 y_{\ell+1}) + \phi(\bar{D}_3 y_{\ell+2})] \\
&\quad + \frac{\varepsilon}{3} [2\phi(\bar{D}_3 y_{N^{**}}) + \phi(\bar{D}_3 y_{N^{**}+1})] + \frac{\varepsilon}{3} [2\phi(\bar{D}_3 y_N) + \phi(\bar{D}_3 y_{N-1})].
\end{aligned} \tag{2.117}$$

The remaining proof is similar to Lemma 8.  $\square$

**Lemma 10.** *For a smooth function  $y$  and a smooth function  $\phi$  whose derivatives are bounded we have*

$$E_{\Omega^*,3}^{a,CB}\{y\} = \varepsilon \sum_{\ell=N^*}^{N^{**}-1} \phi(3\bar{D}_1 y_\ell) = \varepsilon \sum_{\ell=N^*}^{N^{**}-1} \phi(3y'(m_\ell)) + O(\varepsilon^2). \quad (2.118)$$

*Proof.* Since,  $\bar{D}_1 y_\ell = \frac{y_{\ell+1} - y_\ell}{\varepsilon} = y'(m_\ell) + O(\varepsilon^2)$ , we have

$$\phi(3\bar{D}_1 y_\ell) = \phi(3y'(m_\ell)) + \phi'(\xi)[3\bar{D}_1 y_\ell - 3y'(m_\ell)], \quad (2.119)$$

where  $\xi$  is between  $3\bar{D}_1 y_\ell$  and  $3y'(m_\ell)$ . Hence,

$$\begin{aligned} |\phi(3\bar{D}_1 y_\ell) - \phi(3y'(m_\ell))| &\leq |\phi'(\xi)[3\bar{D}_1 y_\ell - 3y'(m_\ell)]| \\ &\leq \max_{\xi} |\phi'(\xi)| |3\bar{D}_1 y_\ell - 3y'(m_\ell)| \\ &\leq c\varepsilon^2. \end{aligned} \quad (2.120)$$

$\square$

Equation (2.104) will be examined in sections as below

$$\begin{aligned} A_{CB} - E_{\Omega_{a_1},3}^a\{y\} &= \varepsilon \sum_{K=(x_1,x_2)}^{(x_{N^*-3},x_{N^*-2})} \phi(3y'(m_K)) - \varepsilon \sum_{\ell=1}^{N^*-3} \phi(\bar{D}_3 y_\ell) \\ &= \varepsilon \sum_{K=(x_1,x_2)}^{(x_{N^*-3},x_{N^*-2})} \phi(3y'(m_K)) - \varepsilon \sum_{\ell=1}^{N^*-5} \phi(3y'(m_{\ell+2})) \\ &\quad - \frac{\varepsilon}{3}[2\phi(\bar{D}_3 y_1) + \phi(\bar{D}_3 y_2)] - \frac{\varepsilon}{3}[2\phi(\bar{D}_3 y_{N^*-3}) + \phi(\bar{D}_3 y_{N^*-4})] \\ &\quad + O(\varepsilon^2) \\ &= \varepsilon \phi(3y'(m_{(x_1,x_2)})) + \varepsilon \phi(3y'(m_{(x_2,x_3)})) + \dots \\ &\quad + \varepsilon \phi(3y'(m_{(x_{N^*-3},x_{N^*-2})})) - \varepsilon \phi(3y'(m_3)) - \varepsilon \phi(3y'(m_4)) \dots \\ &\quad - \varepsilon \phi(3y'(m_{N^*-3})) - \frac{\varepsilon}{3}[2\phi(\bar{D}_3 y_1) + \phi(\bar{D}_3 y_2)] \\ &\quad - \frac{\varepsilon}{3}[2\phi(\bar{D}_3 y_{N^*-3}) + \phi(\bar{D}_3 y_{N^*-4})] + O(\varepsilon^2) \\ &= \varepsilon \phi(3y'(m_{(x_1,x_2)})) + \varepsilon \phi(3y'(m_{(x_2,x_3)})) \\ &\quad - \frac{\varepsilon}{3}[2\phi(\bar{D}_3 y_1) + \phi(\bar{D}_3 y_2)] - \frac{\varepsilon}{3}[2\phi(\bar{D}_3 y_{N^*-3}) + \phi(\bar{D}_3 y_{N^*-4})] \\ &\quad + O(\varepsilon^2), \end{aligned} \quad (2.121)$$

where Lemma 8 was applied. Further,

$$\begin{aligned}
B_{CB} - E_{\Gamma_1,3}^D\{y\} = & \varepsilon \sum_{K=(x_{N^*-2}, x_{N^*-1})}^{(x_{N^*}, x_{N^*+1})} \phi(3y'(m_K)) - \frac{2\varepsilon}{3} \phi(\bar{D}_3 y_{N^*-2}) - \frac{\varepsilon}{3} \phi(\bar{D}_3 y_{N^*-1}) \\
& + \frac{1}{3} \phi' \left( \frac{3}{2} \left\{ \frac{y_{N^*+1} - y_{N^*-2}}{3\varepsilon} + \frac{y_{N^*+1} - y_{N^*}}{\varepsilon} \right\} \right) [y_{N^*-2} + 2y_{N^*+1} \\
& - 3y_{N^*}] + \frac{1}{3} \phi' \left( \frac{3}{2} \left\{ \frac{y_{N^*+2} - y_{N^*-1}}{3\varepsilon} + \frac{y_{N^*+1} - y_{N^*}}{\varepsilon} \right\} \right) [2y_{N^*-1} \\
& + y_{N^*+2} - 3y_{N^*}] \\
= & \varepsilon \phi(3y'(m_{(x_{N^*-2}, x_{N^*-1})})) + \varepsilon \phi(3y'(m_{(x_{N^*-1}, x_{N^*})})) \\
& + \varepsilon \phi(3y'(m_{(x_{N^*}, x_{N^*+1})})) - \frac{2\varepsilon}{3} \phi(\bar{D}_3 y_{N^*-2}) - \frac{\varepsilon}{3} \phi(\bar{D}_3 y_{N^*-1}) \\
& + \frac{1}{3} \phi' \left( \frac{3}{2} \left\{ \frac{y_{N^*+1} - y_{N^*-2}}{3\varepsilon} + \frac{y_{N^*+1} - y_{N^*}}{\varepsilon} \right\} \right) [y_{N^*-2} + 2y_{N^*+1} \\
& - 3y_{N^*}] + \frac{1}{3} \phi' \left( \frac{3}{2} \left\{ \frac{y_{N^*+2} - y_{N^*-1}}{3\varepsilon} + \frac{y_{N^*+1} - y_{N^*}}{\varepsilon} \right\} \right) [2y_{N^*-1} \\
& + y_{N^*+2} - 3y_{N^*}],
\end{aligned} \tag{2.122}$$

and

$$\begin{aligned}
\Gamma_{CB} - E_{\Omega_*,3}^{a,CB}\{y\} = & \varepsilon \sum_{K=(x_{N^*+1}, x_{N^*+2})}^{(x_{N^{**}-2}, x_{N^{**}-1})} \phi(3y'(m_K)) - \varepsilon \sum_{\ell=N^*}^{N^{**}-1} \phi(3y'(m_\ell)) \\
= & \varepsilon \phi(3y'(m_{(x_{N^*+1}, x_{N^*+2})})) + \varepsilon \phi(3y'(m_{(x_{N^*+2}, x_{N^*+3})})) + \cdots \\
& + \varepsilon \phi(3y'(m_{(x_{N^{**}-2}, x_{N^{**}-1})})) - \varepsilon \phi(3y'(m_{N^*})) - \varepsilon \phi(3y'(m_{N^*+1})) \\
& - \cdots - \varepsilon \phi(3y'(m_{N^{**}-1})) + O(\varepsilon^2) \\
= & -\varepsilon \phi(3y'(m_{N^*})) - \varepsilon \phi(3y'(m_{N^{**}-1})) + O(\varepsilon^2),
\end{aligned} \tag{2.123}$$

where Lemma 10 was applied. Similarly,

$$\begin{aligned}
D_{CB} - E_{\Gamma_2,2}\{y\} = & \varepsilon \sum_{K=(x_{N^{**}-1}, x_{N^{**}})}^{(x_{N^{**}}, x_{N^{**}+1})} \phi(3y'(m_K)) - \frac{2\varepsilon}{3} \phi(\bar{D}_3 y_{N^{**}-2}) \\
& + \frac{1}{3} \phi' \left( \frac{3}{2} \left\{ \frac{y_{N^{**}} - y_{N^{**}-1}}{\varepsilon} + \frac{y_{N^{**}+1} - y_{N^{**}-2}}{3\varepsilon} \right\} \right) [3y_{N^{**}} \\
& - y_{N^{**}-2} - 2y_{N^{**}+1}] - \frac{\varepsilon}{3} \phi(\bar{D}_3 y_{N^{**}-1}) \\
& + \frac{1}{3} \phi' \left( \frac{3}{2} \left\{ \frac{y_{N^{**}} - y_{N^{**}-1}}{\varepsilon} + \frac{y_{N^{**}+2} - y_{N^{**}-1}}{3\varepsilon} \right\} \right) [3y_{N^{**}} \\
& - 2y_{N^{**}-1} - y_{N^{**}+2}] \\
= & \varepsilon \phi(2y'(m_{(x_{N^{**}-1}, x_{N^{**}})})) + \varepsilon \phi(3y'(m_{(x_{N^{**}}, x_{N^{**}+1})})) \\
& - \frac{2\varepsilon}{3} \phi(\bar{D}_3 y_{N^{**}-2}) - \frac{\varepsilon}{3} \phi(\bar{D}_3 y_{N^{**}-1}) \\
& + \frac{1}{3} \phi' \left( \frac{3}{2} \left\{ \frac{y_{N^{**}} - y_{N^{**}-1}}{\varepsilon} + \frac{y_{N^{**}+1} - y_{N^{**}-2}}{3\varepsilon} \right\} \right) [3y_{N^{**}} \\
& - y_{N^{**}-2} - 2y_{N^{**}+1}] \\
& + \frac{1}{3} \phi' \left( \frac{3}{2} \left\{ \frac{y_{N^{**}} - y_{N^{**}-1}}{\varepsilon} + \frac{y_{N^{**}+2} - y_{N^{**}-1}}{3\varepsilon} \right\} \right) [3y_{N^{**}} \\
& - 2y_{N^{**}-1} - y_{N^{**}+2}],
\end{aligned} \tag{2.124}$$

and,

$$\begin{aligned}
G_{CB} - E_{\Omega_{a_2},3}^a\{y\} = & \varepsilon \sum_{K=(x_{N^{**}+1}, x_{N^{**}+2})}^{(x_N, x_{N+1})} \phi(3y'(m_K)) - \varepsilon \sum_{\ell=N^{**}}^N \phi(\bar{D}_3 y_\ell) \\
= & \varepsilon \sum_{K=(x_{N^{**}+1}, x_{N^{**}+2})}^{(x_N, x_{N+1})} \phi(3y'(m_K)) - \varepsilon \sum_{\ell=N^{**}}^{N-2} \phi(3y'(m_{\ell+2})) \\
& - \frac{\varepsilon}{3} [2\phi(\bar{D}_3 y_{N^{**}}) + \phi(\bar{D}_3 y_{N^{**}+1})] \\
& - \frac{\varepsilon}{3} [2\phi(\bar{D}_3 y_N) + \phi(\bar{D}_3 y_{N-1})] + O(\varepsilon^2) \\
= & \varepsilon \phi(3y'(m_{(x_{N^{**}+1}, x_{N^{**}+2})})) - \frac{\varepsilon}{3} [2\phi(\bar{D}_3 y_{N^{**}}) + \phi(\bar{D}_3 y_{N^{**}+1})] \\
& - \frac{\varepsilon}{3} [2\phi(\bar{D}_3 y_N) + \phi(\bar{D}_3 y_{N-1})] + O(\varepsilon^2),
\end{aligned} \tag{2.125}$$



where Lemma 9 was applied. Therefore, it is easy to see that,

$$\begin{aligned}
\Phi_3^{CB}(y) - \mathcal{E}_3^D\{y\} = & \varepsilon\phi(3y'(m_{(x_1, x_2)})) + \varepsilon\phi(3y'(m_{(x_2, x_3)})) - \frac{\varepsilon}{3}[2\phi(\bar{D}_3y_1) + \phi(\bar{D}_3y_2)] \\
& - \frac{\varepsilon}{3}[2\phi(\bar{D}_3y_{N^*-3}) + \phi(\bar{D}_3y_{N^*-4})] + \varepsilon\phi(3y'(m_{(x_{N^*-2}, x_{N^*-1})})) \\
& + \varepsilon\phi(3y'(m_{(x_{N^*-1}, x_{N^*})})) - \frac{2\varepsilon}{3}\phi(\bar{D}_3y_{N^*-2}) - \frac{\varepsilon}{3}\phi(\bar{D}_3y_{N^*-1}) \\
& + \frac{1}{3}\phi'\left(\frac{3}{2}\left\{\frac{y_{N^*+1} - y_{N^*-2}}{3\varepsilon} + \frac{y_{N^*+1} - y_{N^*}}{\varepsilon}\right\}\right)[y_{N^*-2} + 2y_{N^*+1} \\
& - 3y_{N^*}] + \frac{1}{3}\phi'\left(\frac{3}{2}\left\{\frac{y_{N^*+2} - y_{N^*-1}}{3\varepsilon} + \frac{y_{N^*+1} - y_{N^*}}{\varepsilon}\right\}\right)[2y_{N^*-1} \\
& + y_{N^*+2} - 3y_{N^*}] + \varepsilon\phi(3y'(m_{(x_{N^{**}}, x_{N^{**}+1})})) - \frac{2\varepsilon}{3}\phi(\bar{D}_3y_{N^{**}-2}) \\
& - \frac{\varepsilon}{3}\phi(\bar{D}_3y_{N^{**}-1}) + \frac{1}{3}\phi'\left(\frac{3}{2}\left\{\frac{y_{N^{**}} - y_{N^{**}-1}}{\varepsilon} + \frac{y_{N^{**}+1} - y_{N^{**}-2}}{3\varepsilon}\right\}\right) \\
& [3y_{N^{**}} - y_{N^{**}-2} - 2y_{N^{**}+1}] \\
& + \frac{1}{3}\phi'\left(\frac{3}{2}\left\{\frac{y_{N^{**}} - y_{N^{**}-1}}{\varepsilon} + \frac{y_{N^{**}+2} - y_{N^{**}-1}}{3\varepsilon}\right\}\right)[3y_{N^{**}} - 2y_{N^{**}-1} \\
& - y_{N^{**}+2}] + \varepsilon\phi(3y'(m_{(x_{N^{**}+1}, x_{N^{**}+2})})) - \frac{\varepsilon}{3}[2\phi(\bar{D}_3y_{N^{**}}) \\
& + \phi(\bar{D}_3y_{N^{**}+1})] - \frac{\varepsilon}{3}[2\phi(\bar{D}_3y_N) + \phi(\bar{D}_3y_{N-1})] + O(\varepsilon^2).
\end{aligned} \tag{2.126}$$

Since  $m_\ell = m_{(x_\ell, x_{\ell+1})}$ , we conclude,

$$\begin{aligned}
\Phi_3^{CB}(y) - \mathcal{E}_3^D\{y\} = & \varepsilon\phi(3y'(m_1)) + \varepsilon\phi(3y'(m_2)) - \frac{\varepsilon}{3}[2\phi(\bar{D}_3y_1) + \phi(\bar{D}_3y_2)] \\
& - \frac{\varepsilon}{3}[2\phi(\bar{D}_3y_{N^*-3}) + \phi(\bar{D}_3y_{N^*-4})] + \varepsilon\phi(3y'(m_{N^*-2})) \\
& + \varepsilon\phi(3y'(m_{N^*-1})) - \frac{2\varepsilon}{3}\phi(\bar{D}_3y_{N^*-2}) - \frac{\varepsilon}{3}\phi(\bar{D}_3y_{N^*-1}) \\
& + \frac{1}{3}\phi'\left(\frac{3}{2}\left\{\frac{y_{N^*+1} - y_{N^*-2}}{3\varepsilon} + \frac{y_{N^*+1} - y_{N^*}}{\varepsilon}\right\}\right)[y_{N^*-2} + 2y_{N^*+1} \\
& - 3y_{N^*}] + \frac{1}{3}\phi'\left(\frac{3}{2}\left\{\frac{y_{N^*+2} - y_{N^*-1}}{3\varepsilon} + \frac{y_{N^*+1} - y_{N^*}}{\varepsilon}\right\}\right)[2y_{N^*-1} \\
& + y_{N^*+2} - 3y_{N^*}] + \varepsilon\phi(3y'(m_{N^{**}})) - \frac{2\varepsilon}{3}\phi(\bar{D}_3y_{N^{**}-2}) \\
& - \frac{\varepsilon}{3}\phi(\bar{D}_3y_{N^{**}-1}) + \frac{1}{3}\phi'\left(\frac{3}{2}\left\{\frac{y_{N^{**}} - y_{N^{**}-1}}{\varepsilon} + \frac{y_{N^{**}+1} - y_{N^{**}-2}}{3\varepsilon}\right\}\right) \\
& [3y_{N^{**}} - y_{N^{**}-2} - 2y_{N^{**}+1}] \\
& + \frac{1}{3}\phi'\left(\frac{3}{2}\left\{\frac{y_{N^{**}} - y_{N^{**}-1}}{\varepsilon} + \frac{y_{N^{**}+2} - y_{N^{**}-1}}{3\varepsilon}\right\}\right)[3y_{N^{**}} - 2y_{N^{**}-1} \\
& - y_{N^{**}+2}] + \varepsilon\phi(3y'(m_{N^{**}+1})) - \frac{\varepsilon}{3}[2\phi(\bar{D}_3y_N) + \phi(\bar{D}_3y_{N-1})] \\
& - \frac{\varepsilon}{3}[2\phi(\bar{D}_3y_{N^{**}}) + \phi(\bar{D}_3y_{N^{**}+1})] + O(\varepsilon^2).
\end{aligned} \tag{2.127}$$

In the following two lemmas we will collect certain terms together and examine their order.

**Lemma 11.** *For a smooth function  $y$  and a smooth function  $\phi$  whose derivatives are bounded we have*

$$\begin{aligned} & |\phi' \left( \frac{3}{2} \left\{ \frac{y_{N^*+1} - y_{N^*-2}}{3\varepsilon} + \frac{y_{N^*+1} - y_{N^*}}{\varepsilon} \right\} \right) [y_{N^*-2} + 2y_{N^*+1} - 3y_{N^*}] \\ & + \phi' \left( \frac{3}{2} \left\{ \frac{y_{N^*+2} - y_{N^*-1}}{3\varepsilon} + \frac{y_{N^*+1} - y_{N^*}}{\varepsilon} \right\} \right) [2y_{N^*-1} + y_{N^*+2} - 3y_{N^*}] \leq O(\varepsilon^2). \end{aligned} \quad (2.128)$$

*Proof.* Since  $\phi' \left( \frac{3}{2} \left\{ \frac{y_{N^*+1} - y_{N^*-2}}{3\varepsilon} + \frac{y_{N^*+1} - y_{N^*}}{\varepsilon} \right\} \right)$  and  $\phi' \left( \frac{3}{2} \left\{ \frac{y_{N^*+2} - y_{N^*-1}}{3\varepsilon} + \frac{y_{N^*+1} - y_{N^*}}{\varepsilon} \right\} \right)$  are bounded (Assumption 3) we will only examine

$$[y_{N^*-2} + 2y_{N^*+1} - 3y_{N^*}] \quad \text{and} \quad [2y_{N^*-1} + y_{N^*+2} - 3y_{N^*}]. \quad (2.129)$$

We will apply a Taylor expansion of  $y_{N^*+2}$ ,  $y_{N^*+1}$ ,  $y_{N^*-2}$  and  $y_{N^*-1}$  around  $y_{N^*}$  as follows

$$\begin{aligned} y_{N^*+2} &= y_{N^*} + 2\varepsilon y'(x_{N^*}) + 2\varepsilon^2 y''(x_{N^*}) + \frac{(2\varepsilon)^3}{3!} y'''(\xi_3) \\ y_{N^*+1} &= y_{N^*} + \varepsilon y'(x_{N^*}) + \frac{\varepsilon^2}{2} y''(x_{N^*}) + \frac{\varepsilon^3}{3!} y'''(\xi_1) \\ y_{N^*-1} &= y_{N^*} - \varepsilon y'(x_{N^*}) + \frac{\varepsilon^2}{2} y''(x_{N^*}) - \frac{\varepsilon^3}{3!} y'''(\xi_2) \\ y_{N^*-2} &= y_{N^*} - 2\varepsilon y'(x_{N^*}) + 2\varepsilon^2 y''(x_{N^*}) - \frac{(2\varepsilon)^3}{3!} y'''(\xi_4), \end{aligned} \quad (2.130)$$

where  $\xi_1 \in (x_{N^*}, x_{N^*+1})$ ,  $\xi_2 \in (x_{N^*-1}, x_{N^*})$ ,  $\xi_3 \in (x_{N^*}, x_{N^*+2})$  and  $\xi_4 \in (x_{N^*-2}, x_{N^*})$ . Therefore, (2.129) becomes

$$\begin{aligned} y_{N^*-2} + 2y_{N^*+1} - 3y_{N^*} &= y_{N^*} - 2\varepsilon y'(x_{N^*}) + 2\varepsilon^2 y''(x_{N^*}) - \frac{(2\varepsilon)^3}{3!} y'''(\xi_4) \\ &\quad + 2y_{N^*} + 2\varepsilon y'(x_{N^*}) + \varepsilon^2 y''(x_{N^*}) + 2\frac{\varepsilon^3}{3!} y'''(\xi_1) - 3y_{N^*} \\ &= 3\varepsilon^2 y''(x_{N^*}) + O(\varepsilon^3), \end{aligned} \quad (2.131)$$

and

$$\begin{aligned} 2y_{N^*-1} + y_{N^*+2} - 3y_{N^*} &= 2y_{N^*} - 2\varepsilon y'(x_{N^*}) + \varepsilon^2 y''(x_{N^*}) - 2\frac{\varepsilon^3}{3!} y'''(\xi_2) \\ &\quad + y_{N^*} + 2\varepsilon y'(x_{N^*}) + 2\varepsilon^2 y''(x_{N^*}) + \frac{(2\varepsilon)^3}{3!} y'''(\xi_3) - 3y_{N^*} \\ &= 3\varepsilon^2 y''(x_{N^*}) + O(\varepsilon^3). \end{aligned} \quad (2.132)$$

Hence,

$$\begin{aligned} & \left| \phi' \left( \frac{3}{2} \left\{ \frac{y_{N^*+1} - y_{N^*-2}}{3\varepsilon} + \frac{y_{N^*+1} - y_{N^*}}{\varepsilon} \right\} \right) [y_{N^*-2} - 2y_{N^*+1} - 3y_{N^*}] \right. \\ & \left. + \phi' \left( \frac{3}{2} \left\{ \frac{y_{N^*+2} - y_{N^*-1}}{3\varepsilon} + \frac{y_{N^*+1} - y_{N^*}}{\varepsilon} \right\} \right) [2y_{N^*-1} - y_{N^*+2} - 3y_{N^*}] \right| \leq O(\varepsilon^2). \end{aligned} \quad (2.133)$$

□

Similarly,

$$\begin{aligned} & \left| \frac{1}{3} \phi' \left( \frac{3}{2} \left\{ \frac{y_{N^{**}} - y_{N^{**}-1}}{\varepsilon} + \frac{y_{N^{**}+1} - y_{N^{**}-2}}{3\varepsilon} \right\} \right) [3y_{N^{**}} - y_{N^{**}-2} - 2y_{N^{**}+1}] \right. \\ & \left. + \frac{1}{3} \phi' \left( \frac{3}{2} \left\{ \frac{y_{N^{**}} - y_{N^{**}-1}}{\varepsilon} + \frac{y_{N^{**}+2} - y_{N^{**}-1}}{3\varepsilon} \right\} \right) [3y_{N^{**}} - 2y_{N^{**}-1} - y_{N^{**}+2}] \right| \\ & \leq O(\varepsilon^2). \end{aligned} \quad (2.134)$$

**Lemma 12.** For a smooth function  $y$  and a smooth function  $\phi$  we have

$$|\varepsilon \phi(3y'(m_{N^*-1})) - \frac{\varepsilon}{3} [\phi(\overline{D}_3 y_{N^*-3}) + \phi(\overline{D}_3 y_{N^*-2}) + \phi(\overline{D}_3 y_{N^*-1})]| \leq O(\varepsilon^2) \quad (2.135)$$

*Proof.* As before,

$$\begin{aligned} \overline{D}_3 y_{N^*-3} + \overline{D}_3 y_{N^*-2} + \overline{D}_3 y_{N^*-1} &= \frac{y_{N^*} - y_{N^*-3}}{\varepsilon} + \frac{y_{N^*+1} - y_{N^*-1}}{\varepsilon} + \frac{y_{N^*+2} - y_{N^*-1}}{\varepsilon} \\ &= \frac{y_{N^*+2} - y_{N^*-3}}{\varepsilon} + \frac{y_{N^*+1} - y_{N^*-2}}{\varepsilon} + \frac{y_{N^*} - y_{N^*-1}}{\varepsilon} \\ &= 5y'(m_{N^*-1}) + 3y'(m_{N^*-1}) + y'(m_{N^*-1}) + O(\varepsilon^2) \\ &= 9y'(m_{N^*-1}) + O(\varepsilon^2), \end{aligned} \quad (2.136)$$

and so

$$\frac{1}{3} (\overline{D}_3 y_{N^*-3} + \overline{D}_3 y_{N^*-2} + \overline{D}_3 y_{N^*-1}) = 3y'(m_{N^*-1}) + O(\varepsilon^2). \quad (2.137)$$

Hence, we use the condition from equation (2.110) to obtain,

$$\begin{aligned} & \left| \frac{\phi(\overline{D}_3 y_{N^*-3}) + \phi(\overline{D}_3 y_{N^*-2}) + \phi(\overline{D}_3 y_{N^*-1})}{3} - \phi \left( \frac{\overline{D}_3 y_{N^*-3} + \overline{D}_3 y_{N^*-2} + \overline{D}_3 y_{N^*-1}}{3} \right) \right| \\ & \leq c\varepsilon^2. \end{aligned} \quad (2.138)$$

Hence, (2.135) holds. □

Similarly,

$$|\varepsilon \phi(3y'(m_{N^*-2})) - \frac{\varepsilon}{3} [\phi(\overline{D}_3 y_{N^*-4}) + \phi(\overline{D}_3 y_{N^*-3}) + \phi(\overline{D}_3 y_{N^*-2})]| \leq O(\varepsilon^2), \quad (2.139)$$

$$|\varepsilon \phi(3y'(m_{N^{**}})) - \frac{\varepsilon}{3} [\phi(\overline{D}_3 y_{N^{**}-2}) + \phi(\overline{D}_3 y_{N^{**}-1}) + \phi(\overline{D}_3 y_{N^{**}})]| \leq O(\varepsilon^2), \quad (2.140)$$

$$|\varepsilon \phi(3y'(m_{N^{**}+1})) - \frac{\varepsilon}{3} [\phi(\overline{D}_3 y_{N^{**}-1}) + \phi(\overline{D}_3 y_{N^{**}}) + \phi(\overline{D}_3 y_{N^{**}+1})]| \leq O(\varepsilon^2). \quad (2.141)$$

We are now ready to prove the main result of this section.

**Theorem 2.** *For a smooth function  $y$  the energy consistency error is of second order as follows*

$$|\Phi_3^{CB}(y) - \mathcal{E}_3^D\{y\}| \leq O(\varepsilon^2). \quad (2.142)$$

*Proof.* By applying Lemmas 11 and 12 and (2.139)-(2.141) to (2.127), the four remaining terms from (2.127) that need to be examined are

$$\varepsilon\phi(3y'(m_2)) - \frac{\varepsilon}{3}[\phi(\overline{D}_3y_1) - \phi(\overline{D}_3y_2) - \phi(\overline{D}_3y_N)]. \quad (2.143)$$

If we apply the periodicity condition,

$$y_{\ell+3+N} - y_{\ell+N} = y_{\ell+3} - y_{\ell}, \quad 1 \leq \ell \leq N, \quad (2.144)$$

to the last term of (2.143) we obtain

$$\phi(\overline{D}_3y_N) = \phi(\overline{D}_3y_0), \quad (2.145)$$

and (2.143) becomes

$$\varepsilon\phi(3y'(m_2)) - \frac{\varepsilon}{3}[\phi(\overline{D}_3y_1) - \phi(\overline{D}_3y_2) - \phi(\overline{D}_3y_0)]. \quad (2.146)$$

By following similar steps to those in the proof of Lemma 12 the following holds

$$|\varepsilon\phi(3y'(m_2)) - \frac{\varepsilon}{3}[\phi(\overline{D}_3y_1) - \phi(\overline{D}_3y_2) - \phi(\overline{D}_3y_0)]| \leq O(\varepsilon^2). \quad (2.147)$$

Therefore,

$$|\Phi_3^{a,CB}(y) - \mathcal{E}_3^D\{y\}| \leq O(\varepsilon^2). \quad (2.148)$$

□

# Chapter 3

## Error Analysis for the First Variation in 1D

### 3.1 Chapter Overview

In this chapter we perform the error analysis for the first variation of the coupled model in comparison to the first variation of the atomistic Cauchy-Born energy in one dimension for  $\eta = 2$ . It is important to access the quality of the approximation of the coupled model at the first variation level because the ghost-force phenomenon appears at this level. The setting for this chapter is the same as in Chapter 2. In Section 3.2 we compute the first variation of the atomistic energy, the atomistic Cauchy-Born energy and the energy on the interfaces. We obtain the first variation of the coupled energy in (3.11). In order to be able to subtract (3.11) from the atomistic Cauchy-Born energy (3.14) which only has  $\overline{D}_1 v_\ell$  terms, the  $\overline{D}_2 v_\ell$  terms in (3.11) have to be converted to  $\overline{D}_1 v_\ell$ . This is done by substituting the splitting  $\overline{D}_2 v_\ell = \overline{D}_1 v_\ell + \overline{D}_1 v_{\ell+1}$  into (3.11) which yields (3.12). In Section 3.3 we subtract the first variation of the coupled energy (3.12) from the first variation of the atomistic Cauchy-Born energy (3.14) and obtain (3.15). Some terms in (3.15) contain  $\overline{D}_1 v_{\ell+1}$  which we convert to  $\overline{D}_1 v_\ell$  by using lemmas 13 and 14 so that we can further simplify the calculations. Then by also applying the periodicity condition we obtain (3.26). We examine the order of these terms and apply Lemma 15 and so some of the terms are of order  $O(\varepsilon^2)$ . The remaining terms that are examined are in (3.33)-(3.36) where some terms are  $O(\varepsilon^2)$  and some are  $O(\varepsilon)$ . Finally, in Theorem 3 on page 59 we show that the variational consistency error was bounded by  $(\varepsilon^2 + \varepsilon^{2-\frac{1}{p}})$  in the discrete  $W^{-1,p}$  norm.

Sections 3.4 and 3.4.1 include the numerical results for the optimisation of the atomistic model and the optimisation of the discontinuous bond volume based coupling method in one dimension for the Lennard-Jones potential and the Morse potential. We ran the program in Python for four different combinations for the external forces which verified the good performance of the coupling method compared to the fully atomistic model.

## 3.2 Variation of Coupled Energy

The setting of the coupled energy and the atomistic energy is the same as in Chapter 2. We will compute the difference between the first variation of the coupled energy and the first variation of the atomistic Cauchy-Born energy as follows

$$\langle D\Phi_2^{a,CB}(y), v \rangle_\varepsilon - \langle D\mathcal{E}_2^D\{y\}, v \rangle_\varepsilon$$

where

$$\begin{aligned} \langle D\mathcal{E}_2^D\{y\}, v \rangle_\varepsilon &= \langle DE_{\Omega_{a_1},2}^a\{y\}, v \rangle_\varepsilon + \langle DE_{\Gamma_{1,2}}^D\{y\}, v \rangle_\varepsilon + \langle DE_{\Omega_{*,2}}^{a,CB}\{y\}, v \rangle_\varepsilon \\ &\quad + \langle DE_{\Gamma_{2,2}}^D\{y\}, v \rangle_\varepsilon + \langle DE_{\Omega_{a_2},2}^a\{y\}, v \rangle_\varepsilon. \end{aligned} \quad (3.1)$$

We will look at each term of (3.1) separately, where the energies in each region have been defined in (2.34) in Section 2.2.4. The first term is as follows

$$\langle DE_{\Omega_{a_1},2}^a\{y\}, v \rangle_\varepsilon = \frac{d}{dt} E_{\Omega_{a_1},2}^a(y + tv)|_{t=0}$$

and

$$\frac{d}{dt} E_{\Omega_{a_1},2}^a(y + tv) = \varepsilon \sum_{\ell=1}^{N^*-2} \frac{d\phi}{dt}(\bar{D}_2(y_\ell + tv_\ell)) = \varepsilon \sum_{\ell=1}^{N^*-2} \phi'(\bar{D}_2(y_\ell + tv_\ell)) \bar{D}_2 v_\ell. \quad (3.2)$$

So,

$$\langle DE_{\Omega_{a_1},2}^a(y), v \rangle_\varepsilon = \varepsilon \sum_{\ell=1}^{N^*-2} \phi'(\bar{D}_2 y_\ell) \bar{D}_2 v_\ell. \quad (3.3)$$

The second term is as follows

$$\langle DE_{\Gamma_{1,2}}^D(y), v \rangle_\varepsilon = \frac{d}{dt} E_{\Gamma_{1,2}}^D(y + tv)|_{t=0} \quad (3.4)$$

and

$$\begin{aligned} \frac{d}{dt} E_{\Gamma_{1,2}}^D(y + tv) &= \frac{d}{dt} \left[ \sum_{\substack{\ell=1 \\ B_{\ell,2} \cap \Gamma_1 \neq \emptyset}}^N \left\{ \frac{\varepsilon}{2} \phi(\bar{D}_2(y_\ell + tv_\ell)) \right. \right. \\ &\quad \left. \left. - \frac{1}{2} \phi'(\{\{2(y^{\ell,2}(x_{\ell+1}) + tv^{\ell,2})'\}\}) \llbracket 2(y^{\ell,2}(x_{\ell+1}) + tv^{\ell,2}) \rrbracket \right\} \right] \\ &= \sum_{\substack{\ell=1 \\ B_{\ell,2} \cap \Gamma_1 \neq \emptyset}}^N \left\{ \frac{\varepsilon}{2} \phi'(\bar{D}_2(y_\ell + tv_\ell)) \bar{D}_2 v_\ell \right. \\ &\quad - \frac{1}{2} \phi''(\{\{2(y^{\ell,2}(x_{\ell+1}) + tv^{\ell,2})'\}\}) \llbracket 2(y^{\ell,2}(x_{\ell+1}) + tv^{\ell,2}) \rrbracket \{\{2(v^{\ell,2})'\}\} \\ &\quad \left. - \frac{1}{2} \phi'(\{\{2(y^{\ell,2}(x_{\ell+1}) + tv^{\ell,2})'\}\}) \llbracket 2v^{\ell,2} \rrbracket \right\}. \end{aligned} \quad (3.5)$$

Hence,

$$\begin{aligned}
\langle DE_{\Gamma_1,2}(y), v \rangle_\varepsilon &= \sum_{\substack{\ell=1 \\ B_{\ell,2} \cap \Gamma_1 \neq \emptyset}}^N \left\{ \frac{\varepsilon}{2} \phi'(\bar{D}_2 y_\ell) \bar{D}_2 v_\ell \right. \\
&\quad - \frac{1}{2} \phi''(\{\{2(y^{\ell,2}(x_{\ell+1}))'\}\}) \llbracket 2(y^{\ell,2}(x_{\ell+1})) \rrbracket \{\{2(v^{\ell,2})'\}\} \\
&\quad \left. - \frac{1}{2} \phi'(\{\{2(y^{\ell,2}(x_{\ell+1}))'\}\}) \llbracket 2v^{\ell,2} \rrbracket \right\} \\
&= \frac{\varepsilon}{2} \phi'(\bar{D}_2 y_{N^*-1}) \bar{D}_2 v_{N^*-1} \\
&\quad - \frac{1}{2} \phi''(\{\{2(y^{N^*-1,2}(x_{N^*}))'\}\}) \llbracket 2(y^{N^*-1,2}(x_{N^*})) \rrbracket \{\{2(v^{N^*-1,2})'\}\} \\
&\quad - \frac{1}{2} \phi'(\{\{2(y^{N^*-1,2}(x_{N^*}))'\}\}) \llbracket 2v^{N^*-1,2} \rrbracket.
\end{aligned} \tag{3.6}$$

By substituting (2.18)-(2.21) into (3.6) we obtain

$$\begin{aligned}
\langle DE_{\Gamma_1,2}(y), v \rangle_\varepsilon &= \frac{\varepsilon}{2} \phi'(\bar{D}_2 y_{N^*-1}) \bar{D}_2 v_{N^*-1} \\
&\quad - \frac{1}{2} \phi''\left(\frac{1}{2} \{2(y^{N^*-1,2}(x_{N^*}))'^- + 2(y^{N^*-1,2}(x_{N^*}))'^+\}\right) \\
&\quad [2(y^{N^*-1,2}(x_{N^*}))^- - 2(y^{N^*-1,2}(x_{N^*}))^+] \{(v^{N^*-1,2})'^- + (v^{N^*-1,2})'^+\} \\
&\quad - \frac{1}{2} \phi'\left(\frac{1}{2} \{2(y^{N^*-1,2}(x_{N^*}))'^- + 2(y^{N^*-1,2}(x_{N^*}))'^+\}\right) \\
&\quad [2(v^{N^*-1,2}(x_{N^*}))^- - 2(v^{N^*-1,2}(x_{N^*}))^+] \\
&= \frac{\varepsilon}{2} \phi'(\bar{D}_2 y_{N^*-1}) \bar{D}_2 v_{N^*-1} - \frac{1}{2} \phi''\left(\frac{y_{N^*+1} - y_{N^*-1}}{x_{N^*+1} - x_{N^*-1}} + \frac{y_{N^*+1} - y_{N^*}}{\varepsilon}\right) \\
&\quad [2y_{N^*-1} + 2\left(\frac{y_{N^*+1} - y_{N^*-1}}{x_{N^*+1} - x_{N^*-1}}\right)(x_{N^*} - x_{N^*-1}) - 2y_{N^*}] \\
&\quad \left[\frac{v_{N^*+1} - v_{N^*-1}}{x_{N^*+1} - x_{N^*-1}} + \frac{v_{N^*+1} - v_{N^*}}{\varepsilon}\right] \\
&\quad - \frac{1}{2} \phi'\left(\frac{y_{N^*+1} - y_{N^*-1}}{x_{N^*+1} - x_{N^*-1}} + \frac{y_{N^*+1} - y_{N^*}}{\varepsilon}\right) [2v_{N^*-1} \\
&\quad + 2\left(\frac{v_{N^*+1} - v_{N^*-1}}{x_{N^*+1} - x_{N^*-1}}\right)(x_{N^*} - x_{N^*-1}) - 2v_{N^*}] \\
&= \frac{\varepsilon}{2} \phi'(\bar{D}_2 y_{N^*-1}) \bar{D}_2 v_{N^*-1} - \frac{1}{2} \phi''\left(\frac{1}{2} \bar{D}_2 y_{N^*-1} + \bar{D}_1 y_{N^*}\right) \\
&\quad [y_{N^*+1} + y_{N^*-1} - 2y_{N^*}] \left[\frac{1}{2} \bar{D}_2 v_{N^*-1} + \bar{D}_1 v_{N^*}\right] \\
&\quad - \frac{1}{2} \phi'\left(\frac{1}{2} \bar{D}_2 y_{N^*-1} + \bar{D}_1 y_{N^*}\right) [v_{N^*+1} + v_{N^*-1} - 2v_{N^*}]
\end{aligned}$$

$$\begin{aligned}
&= \frac{\varepsilon}{2} \phi'(\bar{D}_2 y_{N^*-1}) \bar{D}_2 v_{N^*-1} - \frac{\varepsilon}{2} \phi''(\frac{1}{2} \bar{D}_2 y_{N^*-1} + \bar{D}_1 y_{N^*}) \\
&\quad [\bar{D}_1 y_{N^*} - \bar{D}_1 y_{N^*-1}] \left[ \frac{1}{2} \bar{D}_1 v_{N^*-1} + \frac{3}{2} \bar{D}_1 v_{N^*} \right] \\
&\quad - \frac{\varepsilon}{2} \phi'(\frac{1}{2} \bar{D}_2 y_{N^*-1} + \bar{D}_1 y_{N^*}) [\bar{D}_1 v_{N^*} - \bar{D}_1 v_{N^*-1}].
\end{aligned} \tag{3.7}$$

By similar computations, we conclude that the first variation of  $E_{\Gamma_{2,2}}$  is

$$\begin{aligned}
\langle DE_{\Gamma_{2,2}}(y), v \rangle_\varepsilon &= \frac{\varepsilon}{2} \phi'(\bar{D}_2 y_{N^{**}-1}) \bar{D}_2 v_{N^{**}-1} - \frac{1}{2} \phi''(\frac{1}{2} \bar{D}_2 y_{N^{**}-1} + \bar{D}_1 y_{N^{**}-1}) \\
&\quad [-2y_{N^{**}} + y_{N^{**}+1} + y_{N^{**}-1}] \left\{ \frac{1}{2} \bar{D}_2 v_{N^{**}-1} + \bar{D}_1 v_{N^{**}-1} \right\} \\
&\quad - \frac{1}{2} \phi'(\frac{1}{2} \bar{D}_2 y_{N^{**}-1} + \bar{D}_1 y_{N^{**}-1}) [-2v_{N^{**}} + v_{N^{**}+1} + v_{N^{**}-1}] \\
&= \frac{\varepsilon}{2} \phi'(\bar{D}_2 y_{N^{**}-1}) \bar{D}_2 v_{N^{**}-1} - \frac{\varepsilon}{2} \phi''(\frac{1}{2} \bar{D}_2 y_{N^{**}-1} + \bar{D}_1 y_{N^{**}-1}) \\
&\quad [-\bar{D}_1 y_{N^{**}-1} + \bar{D}_1 y_{N^{**}}] \left\{ \frac{1}{2} \bar{D}_2 v_{N^{**}-1} + \bar{D}_1 v_{N^{**}-1} \right\} \\
&\quad - \frac{\varepsilon}{2} \phi'(\frac{1}{2} \bar{D}_2 y_{N^{**}-1} + \bar{D}_1 y_{N^{**}-1}) [-\bar{D}_1 v_{N^{**}-1} + \bar{D}_1 v_{N^{**}}].
\end{aligned} \tag{3.8}$$

Noting (2.34) we have

$$\langle DE_{\Omega_{*,2}}^{a,CB}(y), v \rangle_\varepsilon = 2\varepsilon \sum_{\ell=N^*}^{N^{**}-1} \phi'(2\bar{D}_1 y_\ell) \bar{D}_1 v_\ell, \tag{3.9}$$

and by similar computations as in (3.2) we obtain

$$\langle DE_{\Omega_{a_2,2}}^a(y), v \rangle_\varepsilon = \varepsilon \sum_{\ell=N^{**}}^N \phi'(\bar{D}_2 y_\ell) \bar{D}_2 v_\ell. \tag{3.10}$$

Therefore, (3.1) becomes

$$\begin{aligned}
\langle D\mathcal{E}_2^D\{y\}, v \rangle_\varepsilon &= \varepsilon \sum_{\ell=1}^{N^*-2} \phi'(\bar{D}_2 y_\ell) \bar{D}_2 v_\ell + \frac{\varepsilon}{2} \phi'(\bar{D}_2 y_{N^*-1}) \bar{D}_2 v_{N^*-1} \\
&\quad - \frac{\varepsilon}{2} \phi''(\frac{1}{2} \bar{D}_2 y_{N^*-1} + \bar{D}_1 y_{N^*}) [\bar{D}_1 y_{N^*} - \bar{D}_1 y_{N^*-1}] \left\{ \frac{1}{2} \bar{D}_1 v_{N^*-1} \right. \\
&\quad \left. + \frac{3}{2} \bar{D}_1 v_{N^*} \right\} - \frac{\varepsilon}{2} \phi'(\frac{1}{2} \bar{D}_2 y_{N^*-1} + \bar{D}_1 y_{N^*}) [\bar{D}_1 v_{N^*} - \bar{D}_1 v_{N^*-1}] \\
&\quad + 2\varepsilon \sum_{\ell=N^*}^{N^{**}-1} \phi'(2\bar{D}_1 y_\ell) \bar{D}_1 v_\ell + \frac{\varepsilon}{2} \phi'(\bar{D}_2 y_{N^{**}-1}) \bar{D}_2 v_{N^{**}-1} \\
&\quad - \frac{\varepsilon}{2} \phi''(\frac{1}{2} \bar{D}_2 y_{N^{**}-1} + \bar{D}_1 y_{N^{**}-1}) [-\bar{D}_1 y_{N^{**}-1} + \bar{D}_1 y_{N^{**}}] \\
&\quad \left\{ \frac{1}{2} \bar{D}_2 v_{N^{**}-1} + \bar{D}_1 v_{N^{**}-1} \right\} - \frac{\varepsilon}{2} \phi'(\frac{1}{2} \bar{D}_2 y_{N^{**}-1} + \bar{D}_1 y_{N^{**}-1}) \\
&\quad [-\bar{D}_1 v_{N^{**}-1} + \bar{D}_1 v_{N^{**}}] + \varepsilon \sum_{\ell=N^{**}}^N \phi'(\bar{D}_2 y_\ell) \bar{D}_2 v_\ell.
\end{aligned} \tag{3.11}$$



We will rewrite equation (3.11) in terms of  $\bar{D}_1 v_\ell$  by substituting  $\bar{D}_2 v_\ell = \bar{D}_1 v_\ell + \bar{D}_1 v_{\ell+1}$  as follows

$$\begin{aligned}
\langle D\mathcal{E}_2^D\{y\}, v \rangle_\varepsilon = & \varepsilon \sum_{\ell=1}^{N^*-2} \phi'(\bar{D}_2 y_\ell) [\bar{D}_1 v_\ell + \bar{D}_1 v_{\ell+1}] + \frac{\varepsilon}{2} \phi'(\bar{D}_2 y_{N^*-1}) [\bar{D}_1 v_{N^*-1} + \bar{D}_1 v_{N^*}] \\
& - \frac{\varepsilon}{2} \phi''(\frac{1}{2} \bar{D}_2 y_{N^*-1} + \bar{D}_1 y_{N^*}) [\bar{D}_1 y_{N^*} - \bar{D}_1 y_{N^*-1}] \left\{ \frac{1}{2} \bar{D}_1 v_{N^*-1} \right. \\
& \left. + \frac{3}{2} \bar{D}_1 v_{N^*} \right\} - \frac{\varepsilon}{2} \phi'(\frac{1}{2} \bar{D}_2 y_{N^*-1} + \bar{D}_1 y_{N^*}) [\bar{D}_1 v_{N^*} - \bar{D}_1 v_{N^*-1}] \\
& + 2\varepsilon \sum_{\ell=N^*}^{N^{**}-1} \phi'(2\bar{D}_1 y_\ell) \bar{D}_1 v_\ell + \frac{\varepsilon}{2} \phi'(\bar{D}_2 y_{N^{**}-1}) [\bar{D}_1 v_{N^{**}-1} + \bar{D}_1 v_{N^{**}}] \\
& - \frac{\varepsilon}{2} \phi''(\frac{1}{2} \bar{D}_2 y_{N^{**}-1} + \bar{D}_1 y_{N^{**}}) [-\bar{D}_1 y_{N^{**}-1} + \bar{D}_1 y_{N^{**}}] \\
& \left\{ \frac{1}{2} \bar{D}_1 v_{N^{**}} + \frac{3}{2} \bar{D}_1 v_{N^{**}-1} \right\} - \frac{\varepsilon}{2} \phi'(\frac{1}{2} \bar{D}_2 y_{N^{**}-1} + \bar{D}_1 y_{N^{**}}) \\
& [-\bar{D}_1 v_{N^{**}-1} + \bar{D}_1 v_{N^{**}}] + \varepsilon \sum_{\ell=N^{**}}^N \phi'(\bar{D}_2 y_\ell) [\bar{D}_1 v_\ell + \bar{D}_1 v_{\ell+1}].
\end{aligned} \tag{3.12}$$

### 3.3 Variation of Continuum Energy and Coupled Energy

The atomistic Cauchy-Born potential energy for  $\eta = 2$  is

$$\Phi_2^{a,CB}(y) = \varepsilon \sum_{\ell=1}^N \phi(2\bar{D}_1 y_\ell), \tag{3.13}$$

and its first variation is

$$\langle D\Phi_2^{a,CB}(y), v \rangle_\varepsilon = 2\varepsilon \sum_{\ell=1}^N \phi'(2\bar{D}_1 y_\ell) \bar{D}_1 v_\ell. \tag{3.14}$$

We will calculate  $\langle D\Phi_2^{CB}(y) - D\mathcal{E}_2^D(y), v \rangle_\varepsilon$  as follows

$$\begin{aligned}
\langle D\Phi_2^{a,CB}(y) - D\mathcal{E}_2^D(y), v \rangle_\varepsilon &= 2\varepsilon \sum_{\ell=1}^N \phi'(2\bar{D}_1 y_\ell) \bar{D}_1 v_\ell \\
&- \varepsilon \sum_{\ell=1}^{N^*-2} \phi'(\bar{D}_2 y_\ell) [\bar{D}_1 v_\ell + \bar{D}_1 v_{\ell+1}] - \frac{\varepsilon}{2} \phi'(\bar{D}_2 y_{N^*-1}) [\bar{D}_1 v_{N^*-1} + \bar{D}_1 v_{N^*}] \\
&+ \frac{\varepsilon}{2} \phi'' \left( \frac{1}{2} \bar{D}_2 y_{N^*-1} + \bar{D}_1 y_{N^*} \right) [\bar{D}_1 y_{N^*} - \bar{D}_1 y_{N^*-1}] \left\{ \frac{1}{2} \bar{D}_1 v_{N^*-1} + \frac{3}{2} \bar{D}_1 v_{N^*} \right\} \\
&+ \frac{\varepsilon}{2} \phi' \left( \frac{1}{2} \bar{D}_2 y_{N^*-1} + \bar{D}_1 y_{N^*} \right) [\bar{D}_1 v_{N^*} - \bar{D}_1 v_{N^*-1}] \\
&- 2\varepsilon \sum_{\ell=N^*}^{N^{**}-1} \phi'(2\bar{D}_1 y_\ell) \bar{D}_1 v_\ell - \frac{\varepsilon}{2} \phi'(\bar{D}_2 y_{N^{**}-1}) [\bar{D}_1 v_{N^{**}-1} + \bar{D}_1 v_{N^{**}}] \\
&+ \frac{\varepsilon}{2} \phi'' \left( \frac{1}{2} \bar{D}_2 y_{N^{**}-1} + \bar{D}_1 y_{N^{**}} \right) [-\bar{D}_1 y_{N^{**}-1} + \bar{D}_1 y_{N^{**}}] \left\{ \frac{1}{2} \bar{D}_1 v_{N^{**}} + \frac{3}{2} \bar{D}_1 v_{N^{**}-1} \right\} \\
&+ \frac{\varepsilon}{2} \phi' \left( \frac{1}{2} \bar{D}_2 y_{N^{**}-1} + \bar{D}_1 y_{N^{**}} \right) [-\bar{D}_1 v_{N^{**}-1} + \bar{D}_1 v_{N^{**}}] \\
&- \varepsilon \sum_{\ell=N^{**}}^N \phi'(\bar{D}_2 y_\ell) [\bar{D}_1 v_\ell + \bar{D}_1 v_{\ell+1}].
\end{aligned} \tag{3.15}$$

We will introduce two lemmas that will help us rewrite the summations with the term  $\bar{D}_1 v_{\ell+1}$  in terms of  $\bar{D}_1 v_\ell$ .

**Lemma 13.** *For a smooth function  $y$  and a smooth function  $\phi$  whose derivatives are bounded we have*

$$\begin{aligned}
\varepsilon \sum_{\ell=1}^{N^*-2} \phi'(\bar{D}_2 y_\ell) [\bar{D}_1 v_\ell + \bar{D}_1 v_{\ell+1}] &= \varepsilon \sum_{\ell=1}^{N^*-2} \{ \phi'(\bar{D}_2 y_\ell) + \phi'(\bar{D}_2 y_{\ell-1}) \} \bar{D}_1 v_\ell \\
&+ \varepsilon \phi'(\bar{D}_2 y_{N^*-2}) \bar{D}_1 v_{N^*-1} - \varepsilon \phi'(\bar{D}_2 y_0) \bar{D}_1 v_1.
\end{aligned} \tag{3.16}$$

*Proof.* Consider

$$\varepsilon \sum_{\ell=1}^{N^*-2} \phi'(\bar{D}_2 y_\ell) [\bar{D}_1 v_\ell + \bar{D}_1 v_{\ell+1}] = \varepsilon \sum_{\ell=1}^{N^*-2} \phi'(\bar{D}_2 y_\ell) \bar{D}_1 v_\ell + \varepsilon \sum_{\ell=1}^{N^*-2} \phi'(\bar{D}_2 y_\ell) \bar{D}_1 v_{\ell+1}. \tag{3.17}$$

In order to change the second sum from  $\bar{D}_1 v_{\ell+1}$  to  $\bar{D}_1 v_\ell$  we change the index from

$\ell$  to  $k = \ell + 1$ . Therefore, the second sum of (3.17) becomes

$$\begin{aligned}
\varepsilon \sum_{\ell=1}^{N^*-2} \phi'(\bar{D}_2 y_\ell) \bar{D}_1 v_{\ell+1} &= \varepsilon \sum_{k=2}^{N^*-1} \phi'(\bar{D}_2 y_{k-1}) \bar{D}_1 v_k \\
&= \varepsilon \sum_{k=2}^{N^*-2} \phi'(\bar{D}_2 y_{k-1}) \bar{D}_1 v_k + \varepsilon \phi'(\bar{D}_2 y_{N^*-2}) \bar{D}_1 v_{N^*-1} \\
&= \varepsilon \sum_{k=1}^{N^*-2} \phi'(\bar{D}_2 y_{k-1}) \bar{D}_1 v_k + \varepsilon \phi'(\bar{D}_2 y_{N^*-2}) \bar{D}_1 v_{N^*-1} \\
&\quad - \varepsilon \phi'(\bar{D}_2 y_0) \bar{D}_1 v_1.
\end{aligned} \tag{3.18}$$

Hence,

$$\begin{aligned}
\varepsilon \sum_{\ell=1}^{N^*-2} \phi'(\bar{D}_2 y_\ell) [\bar{D}_1 v_\ell + \bar{D}_1 v_{\ell+1}] &= \varepsilon \sum_{\ell=1}^{N^*-2} \{\phi'(\bar{D}_2 y_\ell) + \phi'(\bar{D}_2 y_{\ell-1})\} \bar{D}_1 v_\ell \\
&\quad + \varepsilon \phi'(\bar{D}_2 y_{N^*-2}) \bar{D}_1 v_{N^*-1} - \varepsilon \phi'(\bar{D}_2 y_0) \bar{D}_1 v_1.
\end{aligned} \tag{3.19}$$

□

Similarly, we have the lemma below.

**Lemma 14.** *For a smooth function  $y$  and a smooth function  $\phi$  whose derivatives are bounded we have*

$$\begin{aligned}
\varepsilon \sum_{\ell=N^{**}}^N \phi'(\bar{D}_2 y_\ell) [\bar{D}_1 v_\ell + \bar{D}_1 v_{\ell+1}] &= \varepsilon \sum_{\ell=N^{**}}^N \{\phi'(\bar{D}_2 y_\ell) + \phi'(\bar{D}_2 y_{\ell-1})\} \bar{D}_1 v_\ell \\
&\quad + \varepsilon \phi'(\bar{D}_2 y_N) \bar{D}_1 v_{N+1} - \varepsilon \phi'(\bar{D}_2 y_{N^{**}-1}) \bar{D}_1 v_{N^{**}}.
\end{aligned} \tag{3.20}$$

*Proof.* Consider

$$\varepsilon \sum_{\ell=N^{**}}^N \phi'(\bar{D}_2 y_\ell) [\bar{D}_1 v_\ell + \bar{D}_1 v_{\ell+1}] = \varepsilon \sum_{\ell=N^{**}}^N \phi'(\bar{D}_2 y_\ell) \bar{D}_1 v_\ell + \varepsilon \sum_{\ell=N^{**}}^N \phi'(\bar{D}_2 y_\ell) \bar{D}_1 v_{\ell+1}. \tag{3.21}$$

As before, we conclude,

$$\begin{aligned}
\varepsilon \sum_{\ell=N^{**}}^N \phi'(\bar{D}_2 y_\ell) [\bar{D}_1 v_\ell + \bar{D}_1 v_{\ell+1}] &= \varepsilon \sum_{\ell=N^{**}}^N \{\phi'(\bar{D}_2 y_\ell) + \phi'(\bar{D}_2 y_{\ell-1})\} \bar{D}_1 v_\ell \\
&\quad + \varepsilon \phi'(\bar{D}_2 y_N) \bar{D}_1 v_{N+1} - \varepsilon \phi'(\bar{D}_2 y_{N^{**}-1}) \bar{D}_1 v_{N^{**}}.
\end{aligned} \tag{3.22}$$

□

We now focus on the following four summations in equation (3.15)

$$\begin{aligned}
& 2\varepsilon \sum_{\ell=1}^N \phi'(2\bar{D}_1 y_\ell) \bar{D}_1 v_\ell - \varepsilon \sum_{\ell=1}^{N^*-2} \phi'(\bar{D}_2 y_\ell) [\bar{D}_1 v_\ell + \bar{D}_1 v_{\ell+1}] \\
& - 2\varepsilon \sum_{\ell=N^*}^{N^{**}-1} \phi'(2\bar{D}_1 y_\ell) \bar{D}_1 v_\ell - \varepsilon \sum_{\ell=N^{**}}^N \phi'(\bar{D}_2 y_\ell) [\bar{D}_1 v_\ell + \bar{D}_1 v_{\ell+1}] := \Lambda.
\end{aligned} \tag{3.23}$$

By applying Lemmas 13 and 14 to (3.23) we obtain

$$\begin{aligned}
\Lambda &= 2\varepsilon \sum_{\ell=1}^N \phi'(2\bar{D}_1 y_\ell) \bar{D}_1 v_\ell - \varepsilon \sum_{\ell=1}^{N^*-2} \{\phi'(\bar{D}_2 y_\ell) + \phi'(\bar{D}_2 y_{\ell-1})\} \bar{D}_1 v_\ell \\
& - \varepsilon \phi'(\bar{D}_2 y_{N^*-2}) \bar{D}_1 v_{N^*-1} + \varepsilon \phi'(\bar{D}_2 y_0) \bar{D}_1 v_1 - 2\varepsilon \sum_{\ell=N^*}^{N^{**}-1} \phi'(2\bar{D}_1 y_\ell) \bar{D}_1 v_\ell \\
& - \varepsilon \sum_{\ell=N^{**}}^N \{\phi'(\bar{D}_2 y_\ell) + \phi'(\bar{D}_2 y_{\ell-1})\} \bar{D}_1 v_\ell - \varepsilon \phi'(\bar{D}_2 y_N) \bar{D}_1 v_{N+1} \\
& + \varepsilon \phi'(\bar{D}_2 y_{N^{**}-1}) \bar{D}_1 v_{N^{**}} \\
& = \varepsilon \sum_{\ell=1}^{N^*-2} \{2\phi'(2\bar{D}_1 y_\ell) - \phi'(\bar{D}_2 y_\ell) - \phi'(\bar{D}_2 y_{\ell-1})\} \bar{D}_1 v_\ell \\
& + 2\varepsilon \phi'(2\bar{D}_1 y_{N^*-1}) \bar{D}_1 v_{N^*-1} - \varepsilon \phi'(\bar{D}_2 y_{N^*-2}) \bar{D}_1 v_{N^*-1} + \varepsilon \phi'(\bar{D}_2 y_0) \bar{D}_1 v_1 \\
& + \varepsilon \sum_{\ell=N^{**}}^N \{2\phi'(2\bar{D}_1 y_\ell) - \phi'(\bar{D}_2 y_\ell) - \phi'(\bar{D}_2 y_{\ell-1})\} \bar{D}_1 v_\ell \\
& - \varepsilon \phi'(\bar{D}_2 y_N) \bar{D}_1 v_{N+1} + \varepsilon \phi'(\bar{D}_2 y_{N^{**}-1}) \bar{D}_1 v_{N^{**}}.
\end{aligned} \tag{3.24}$$

If we apply the periodicity condition then  $\varepsilon \phi'(\bar{D}_2 y_N) \bar{D}_1 v_{N+1} = \varepsilon \phi'(\bar{D}_2 y_0) \bar{D}_1 v_1$ , and hence

$$\begin{aligned}
\Lambda &= \varepsilon \sum_{\ell=1}^{N^*-2} \{2\phi'(2\bar{D}_1 y_\ell) - \phi'(\bar{D}_2 y_\ell) - \phi'(\bar{D}_2 y_{\ell-1})\} \bar{D}_1 v_\ell \\
& + \varepsilon \sum_{\ell=N^{**}}^N \{2\phi'(2\bar{D}_1 y_\ell) - \phi'(\bar{D}_2 y_\ell) - \phi'(\bar{D}_2 y_{\ell-1})\} \bar{D}_1 v_\ell \\
& + 2\varepsilon \phi'(2\bar{D}_1 y_{N^*-1}) \bar{D}_1 v_{N^*-1} - \varepsilon \phi'(\bar{D}_2 y_{N^*-2}) \bar{D}_1 v_{N^*-1} + \varepsilon \phi'(\bar{D}_2 y_{N^{**}-1}) \bar{D}_1 v_{N^{**}}.
\end{aligned} \tag{3.25}$$

Therefore, (3.15) becomes

$$\begin{aligned}
\langle D\Phi_2^{CB}(y) - D\mathcal{E}_2^D(y), v \rangle_\varepsilon &= \varepsilon \sum_{\ell=1}^{N^*-2} \{2\phi'(2\bar{D}_1 y_\ell) - \phi'(\bar{D}_2 y_\ell) - \phi'(\bar{D}_2 y_{\ell-1})\} \bar{D}_1 v_\ell \\
&+ \varepsilon \sum_{\ell=N^{**}}^N \{2\phi'(2\bar{D}_1 y_\ell) - \phi'(\bar{D}_2 y_\ell) - \phi'(\bar{D}_2 y_{\ell-1})\} \bar{D}_1 v_\ell \\
&+ 2\varepsilon \phi'(2\bar{D}_1 y_{N^*-1}) \bar{D}_1 v_{N^*-1} - \varepsilon \phi'(\bar{D}_2 y_{N^*-2}) \bar{D}_1 v_{N^*-1} + \varepsilon \phi'(\bar{D}_2 y_{N^{**}-1}) \bar{D}_1 v_{N^{**}} \\
&- \frac{\varepsilon}{2} \phi'(\bar{D}_2 y_{N^*-1}) [\bar{D}_1 v_{N^*-1} + \bar{D}_1 v_{N^*}] \\
&+ \frac{\varepsilon}{2} \phi''(\frac{1}{2} \bar{D}_2 y_{N^*-1} + \bar{D}_1 y_{N^*}) [\bar{D}_1 y_{N^*} - \bar{D}_1 y_{N^*-1}] \left\{ \frac{1}{2} \bar{D}_1 v_{N^*-1} + \frac{3}{2} \bar{D}_1 v_{N^*} \right\} \\
&+ \frac{\varepsilon}{2} \phi'(\frac{1}{2} \bar{D}_2 y_{N^*-1} + \bar{D}_1 y_{N^*}) [\bar{D}_1 v_{N^*} - \bar{D}_1 v_{N^*-1}] \\
&- \frac{\varepsilon}{2} \phi'(\bar{D}_2 y_{N^{**}-1}) [\bar{D}_1 v_{N^{**}-1} + \bar{D}_1 v_{N^{**}}] \\
&+ \frac{\varepsilon}{2} \phi''(\frac{1}{2} \bar{D}_2 y_{N^{**}-1} + \bar{D}_1 y_{N^{**}-1}) [-\bar{D}_1 y_{N^{**}-1} + \bar{D}_1 y_{N^{**}}] \left\{ \frac{1}{2} \bar{D}_1 v_{N^{**}} + \frac{3}{2} \bar{D}_1 v_{N^{**}-1} \right\} \\
&+ \frac{\varepsilon}{2} \phi'(\frac{1}{2} \bar{D}_2 y_{N^{**}-1} + \bar{D}_1 y_{N^{**}-1}) [-\bar{D}_1 v_{N^{**}-1} + \bar{D}_1 v_{N^{**}}].
\end{aligned} \tag{3.26}$$

We will examine the order of the terms in (3.26). The following lemma proves that the two summations in (3.26) are of order  $O(\varepsilon^2)$

**Lemma 15.** *For a smooth function  $y$  and a smooth function  $\phi$  whose derivative is bounded we have*

$$|2\phi'(2\bar{D}_1 y_\ell) - \phi'(\bar{D}_2 y_\ell) - \phi'(\bar{D}_2 y_{\ell-1})| \leq O(\varepsilon^2). \tag{3.27}$$

*Proof.* Let  $m_\ell$  denote the middle point between  $x_\ell$  and  $x_{\ell+1}$ , then

$$\begin{aligned}
\bar{D}_2 y_\ell + \bar{D}_2 y_{\ell-1} &= \frac{y_{\ell+2} - y_\ell}{\varepsilon} + \frac{y_{\ell+1} - y_{\ell-1}}{\varepsilon} \\
&= \frac{y_{\ell+2} - y_{\ell-1}}{\varepsilon} + \frac{y_{\ell+1} - y_\ell}{\varepsilon} \\
&= 3y'(m_\ell) + y'(m_\ell) + O(\varepsilon^2) \\
&= 4y'(m_\ell) + O(\varepsilon^2).
\end{aligned} \tag{3.28}$$

Hence,

$$\frac{1}{2}(\bar{D}_2 y_\ell + \bar{D}_2 y_{\ell-1}) = 2y'(m_\ell) + O(\varepsilon^2). \tag{3.29}$$

Therefore, using condition (2.42) we obtain

$$\left| \frac{\phi(\bar{D}_2 y_\ell) + \phi(\bar{D}_2 y_{\ell-1})}{2} - \phi\left(\frac{\bar{D}_2 y_\ell + \bar{D}_2 y_{\ell-1}}{2}\right) \right| \leq c\varepsilon^2. \tag{3.30}$$

If we use the Taylor expansion of  $\phi\left(\frac{\bar{D}_2 y_\ell + \bar{D}_2 y_{\ell-1}}{2}\right)$  around  $2y'(m_\ell)$  then

$$\phi\left(\frac{\bar{D}_2 y_\ell + \bar{D}_2 y_{\ell-1}}{2}\right) = \phi(2y'(m_\ell)) + \phi'(\xi) \left[ \frac{\bar{D}_2 y_\ell + \bar{D}_2 y_{\ell-1}}{2} - 2y'(m_\ell) \right]. \tag{3.31}$$

Hence,

$$\begin{aligned}
\left| \phi\left(\frac{\bar{D}_2 y_\ell + \bar{D}_2 y_{\ell-1}}{2}\right) - \phi(2y'(m_\ell)) \right| &\leq \left| \phi'(\xi) \left[ \frac{\bar{D}_2 y_\ell + \bar{D}_2 y_{\ell-1}}{2} - 2y'(m_\ell) \right] \right| \\
&\leq \max_{\xi} |\phi'(\xi)| \left| \frac{\bar{D}_2 y_\ell + \bar{D}_2 y_{\ell-1}}{2} - 2y'(m_\ell) \right| \\
&\leq c\varepsilon^2, \quad c \in \mathbb{R}.
\end{aligned} \tag{3.32}$$

□

The remaining terms we have to examine from (3.26) are the coefficients for  $\bar{D}_1 v_{N^*-1}$ ,  $\bar{D}_1 v_{N^*}$ ,  $\bar{D}_1 v_{N^{**}-1}$  and  $\bar{D}_1 v_{N^{**}}$ .

For  $\bar{D}_1 v_{N^*-1}$ :

$$\begin{aligned}
&2\varepsilon\phi'(2\bar{D}_1 y_{N^*-1}) - \varepsilon\phi'(\bar{D}_2 y_{N^*-2}) - \frac{\varepsilon}{2}\phi'(\bar{D}_2 y_{N^*-1}) \\
&+ \frac{\varepsilon}{4}\phi''\left(\frac{1}{2}\bar{D}_2 y_{N^*-1} + \bar{D}_1 y_{N^*}\right)[\bar{D}_1 y_{N^*} - \bar{D}_1 y_{N^*-1}] - \frac{\varepsilon}{2}\phi'\left(\frac{1}{2}\bar{D}_2 y_{N^*-1} + \bar{D}_1 y_{N^*}\right).
\end{aligned} \tag{3.33}$$

For  $\bar{D}_1 v_{N^*}$ :

$$\begin{aligned}
&-\frac{\varepsilon}{2}\phi'(\bar{D}_2 y_{N^*-1}) + \frac{3\varepsilon}{4}\phi''\left(\frac{1}{2}\bar{D}_2 y_{N^*-1} + \bar{D}_1 y_{N^*}\right)[\bar{D}_1 y_{N^*} - \bar{D}_1 y_{N^*-1}] \\
&+ \frac{\varepsilon}{2}\phi'\left(\frac{1}{2}\bar{D}_2 y_{N^*-1} + \bar{D}_1 y_{N^*}\right).
\end{aligned} \tag{3.34}$$

For  $\bar{D}_1 v_{N^{**}-1}$ :

$$\begin{aligned}
&-\frac{\varepsilon}{2}\phi'(\bar{D}_2 y_{N^{**}-1}) + \frac{3\varepsilon}{4}\phi''\left(\frac{1}{2}\bar{D}_2 y_{N^{**}-1} + \bar{D}_1 y_{N^{**}-1}\right)[-\bar{D}_1 y_{N^{**}-1} + \bar{D}_1 y_{N^{**}}] \\
&+ \frac{\varepsilon}{2}\phi'\left(\frac{1}{2}\bar{D}_2 y_{N^{**}-1} + \bar{D}_1 y_{N^{**}-1}\right).
\end{aligned} \tag{3.35}$$

For  $\bar{D}_1 v_{N^{**}}$ :

$$\begin{aligned}
&\frac{\varepsilon}{2}\phi'(\bar{D}_2 y_{N^{**}-1}) + \frac{\varepsilon}{4}\phi''\left(\frac{1}{2}\bar{D}_2 y_{N^{**}-1} + \bar{D}_1 y_{N^{**}-1}\right)[-\bar{D}_1 y_{N^{**}-1} + \bar{D}_1 y_{N^{**}}] \\
&-\frac{\varepsilon}{2}\phi'\left(\frac{1}{2}\bar{D}_2 y_{N^{**}-1} + \bar{D}_1 y_{N^{**}-1}\right).
\end{aligned} \tag{3.36}$$

We will consider each one separately. The coefficient for  $\bar{D}_1 v_{N^*-1}$  is

$$\begin{aligned}
&2\varepsilon\phi'(2\bar{D}_1 y_{N^*-1}) - \varepsilon\phi'(\bar{D}_2 y_{N^*-2}) - \varepsilon\phi'(\bar{D}_2 y_{N^*-1}) + \frac{\varepsilon}{2}\phi'(\bar{D}_2 y_{N^*-1}) \\
&+ \frac{\varepsilon}{4}\phi''\left(\frac{1}{2}\bar{D}_2 y_{N^*-1} + \bar{D}_1 y_{N^*}\right)[\bar{D}_1 y_{N^*} - \bar{D}_1 y_{N^*-1}] - \frac{\varepsilon}{2}\phi'\left(\frac{1}{2}\bar{D}_2 y_{N^*-1} + \bar{D}_1 y_{N^*}\right).
\end{aligned} \tag{3.37}$$

The first three terms are of order  $O(\varepsilon^2)$  due to Lemma 15 and hence we only have to examine

$$\begin{aligned}
&\frac{\varepsilon}{2}\phi'(\bar{D}_2 y_{N^*-1}) + \frac{\varepsilon}{4}\phi''\left(\frac{1}{2}\bar{D}_2 y_{N^*-1} + \bar{D}_1 y_{N^*}\right)[\bar{D}_1 y_{N^*} - \bar{D}_1 y_{N^*-1}] \\
&-\frac{\varepsilon}{2}\phi'\left(\frac{1}{2}\bar{D}_2 y_{N^*-1} + \bar{D}_1 y_{N^*}\right).
\end{aligned} \tag{3.38}$$

We will expand  $\phi'(\bar{D}_2 y_{N^*-1})$  around  $(\frac{1}{2}\bar{D}_2 y_{N^*-1} + \bar{D}_1 y_{N^*})$  as follows

$$\begin{aligned} \phi'(\bar{D}_2 y_{N^*-1}) &= \phi'(\frac{1}{2}\bar{D}_2 y_{N^*-1} + \bar{D}_1 y_{N^*}) + \frac{1}{2}\phi''(\frac{1}{2}\bar{D}_2 y_{N^*-1} + \bar{D}_1 y_{N^*})(\bar{D}_1 y_{N^*-1} \\ &\quad - \bar{D}_1 y_{N^*}) + \frac{1}{8}\phi'''(\frac{1}{2}\bar{D}_2 y_{N^*-1} + \bar{D}_1 y_{N^*})(\bar{D}_1 y_{N^*-1} - \bar{D}_1 y_{N^*})^2 \\ &\quad + O\left(\left(\frac{\bar{D}_1 y_{N^*-1} - \bar{D}_1 y_{N^*}}{2}\right)^3\right), \end{aligned} \quad (3.39)$$

where  $\frac{1}{2}(\bar{D}_1 y_{N^*-1} - \bar{D}_1 y_{N^*}) = \bar{D}_2 y_{N^*-1} - (\frac{1}{2}\bar{D}_2 y_{N^*-1} + \bar{D}_1 y_{N^*})$ . Hence,

$$\begin{aligned} &\frac{\varepsilon}{2}\phi'(\bar{D}_2 y_{N^*-1}) + \frac{\varepsilon}{4}\phi''(\frac{1}{2}\bar{D}_2 y_{N^*-1} + \bar{D}_1 y_{N^*})[\bar{D}_1 y_{N^*} - \bar{D}_1 y_{N^*-1}] \\ &\quad - \frac{\varepsilon}{2}\phi'(\frac{1}{2}\bar{D}_2 y_{N^*-1} + \bar{D}_1 y_{N^*}) \\ &= \frac{\varepsilon}{2}\phi'(\frac{1}{2}\bar{D}_2 y_{N^*-1} + \bar{D}_1 y_{N^*}) + \frac{\varepsilon}{4}\phi''(\frac{1}{2}\bar{D}_2 y_{N^*-1} + \bar{D}_1 y_{N^*})(\bar{D}_1 y_{N^*-1} - \bar{D}_1 y_{N^*}) \\ &\quad + \frac{\varepsilon}{16}\phi'''(\frac{1}{2}\bar{D}_2 y_{N^*-1} + \bar{D}_1 y_{N^*})(\bar{D}_1 y_{N^*-1} - \bar{D}_1 y_{N^*})^2 + O\left(\left(\frac{\bar{D}_1 y_{N^*-1} - \bar{D}_1 y_{N^*}}{2}\right)^3\right) \\ &\quad - \frac{\varepsilon}{2}\phi'(\frac{1}{2}\bar{D}_2 y_{N^*-1} + \bar{D}_1 y_{N^*}) + \frac{\varepsilon}{4}\phi''(\frac{1}{2}\bar{D}_2 y_{N^*-1} + \bar{D}_1 y_{N^*})(\bar{D}_1 y_{N^*} - \bar{D}_1 y_{N^*-1}) \\ &= \frac{\varepsilon}{16}\phi'''(\frac{1}{2}\bar{D}_2 y_{N^*-1} + \bar{D}_1 y_{N^*})(\bar{D}_1 y_{N^*-1} - \bar{D}_1 y_{N^*})^2 + O\left(\left(\frac{\bar{D}_1 y_{N^*-1} - \bar{D}_1 y_{N^*}}{2}\right)^3\right). \end{aligned} \quad (3.40)$$

We need to check the order of  $\bar{D}_1 y_{N^*-1} - \bar{D}_1 y_{N^*}$  using Taylor expansions of  $y_{N^*+1}$  and  $y_{N^*-1}$  around  $y_{N^*}$

$$\begin{aligned} y_{N^*+1} &= y_{N^*} + \varepsilon y'(x_{N^*}) + \frac{\varepsilon^2}{2}y''(x_{N^*}) + \frac{\varepsilon^3}{3!}y'''(\xi_1), \\ y_{N^*-1} &= y_{N^*} - \varepsilon y'(x_{N^*}) + \frac{\varepsilon^2}{2}y''(x_{N^*}) - \frac{\varepsilon^3}{3!}y'''(\xi_2), \end{aligned} \quad (3.41)$$

where  $\xi_1 \in (x_{N^*}, x_{N^*+1})$  and  $\xi_2 \in (x_{N^*-1}, x_{N^*})$ . Therefore,

$$\bar{D}_1 y_{N^*-1} - \bar{D}_1 y_{N^*} = \frac{2y_{N^*} - y_{N^*+1} - y_{N^*-1}}{\varepsilon} = -\varepsilon y''(x_{N^*}) + O(\varepsilon^3), \quad (3.42)$$

and hence the coefficient (3.33) of  $\bar{D}_1 v_{N^*-1}$  is of order  $O(\varepsilon^2)$ . For  $\bar{D}_1 v_{N^*}$  the coefficient is

$$\begin{aligned} &-\frac{\varepsilon}{2}\phi'(\bar{D}_2 y_{N^*-1}) + \frac{3\varepsilon}{4}\phi''(\frac{1}{2}\bar{D}_2 y_{N^*-1} + \bar{D}_1 y_{N^*})[\bar{D}_1 y_{N^*} - \bar{D}_1 y_{N^*-1}] \\ &\quad + \frac{\varepsilon}{2}\phi'(\frac{1}{2}\bar{D}_2 y_{N^*-1} + \bar{D}_1 y_{N^*}). \end{aligned} \quad (3.43)$$

We will use the Taylor expansion of  $\phi'(\bar{D}_2 y_{N^*-1})$  around  $(\frac{1}{2}\bar{D}_2 y_{N^*-1} + \bar{D}_1 y_{N^*})$  and

substitute it into (3.43) as follows

$$\begin{aligned}
& -\frac{\varepsilon}{2}\phi'(\bar{D}_2 y_{N^*-1}) + \frac{3\varepsilon}{4}\phi''(\frac{1}{2}\bar{D}_2 y_{N^*-1} + \bar{D}_1 y_{N^*})[\bar{D}_1 y_{N^*} - \bar{D}_1 y_{N^*-1}] \\
& + \frac{\varepsilon}{2}\phi'(\frac{1}{2}\bar{D}_2 y_{N^*-1} + \bar{D}_1 y_{N^*}) \\
& = -\frac{\varepsilon}{2}\phi'(\frac{1}{2}\bar{D}_2 y_{N^*-1} + \bar{D}_1 y_{N^*}) - \frac{\varepsilon}{4}\phi''(\frac{1}{2}\bar{D}_2 y_{N^*-1} + \bar{D}_1 y_{N^*})(\bar{D}_1 y_{N^*-1} - \bar{D}_1 y_{N^*}) \\
& - \frac{\varepsilon}{16}\phi'''(\frac{1}{2}\bar{D}_2 y_{N^*-1} + \bar{D}_1 y_{N^*})(\bar{D}_1 y_{N^*-1} - \bar{D}_1 y_{N^*})^2 + O\left(\left(\frac{\bar{D}_1 y_{N^*-1} - \bar{D}_1 y_{N^*}}{2}\right)^3\right) \\
& + \frac{\varepsilon}{2}\phi'(\frac{1}{2}\bar{D}_2 y_{N^*-1} + \bar{D}_1 y_{N^*}) + \frac{3\varepsilon}{4}\phi''(\frac{1}{2}\bar{D}_2 y_{N^*-1} + \bar{D}_1 y_{N^*})(\bar{D}_1 y_{N^*} - \bar{D}_1 y_{N^*-1}) \\
& = -\varepsilon\phi''(\frac{1}{2}\bar{D}_2 y_{N^*-1} + \bar{D}_1 y_{N^*})(\bar{D}_1 y_{N^*-1} - \bar{D}_1 y_{N^*}) \\
& - \frac{\varepsilon}{16}\phi'''(\frac{1}{2}\bar{D}_2 y_{N^*-1} + \bar{D}_1 y_{N^*})(\bar{D}_1 y_{N^*-1} - \bar{D}_1 y_{N^*})^2 + O\left(\left(\frac{\bar{D}_1 y_{N^*-1} - \bar{D}_1 y_{N^*}}{2}\right)^3\right). \tag{3.44}
\end{aligned}$$

The order of  $\bar{D}_1 y_{N^*-1} - \bar{D}_1 y_{N^*}$  is  $O(\varepsilon)$  and hence the order of the coefficient of  $\bar{D}_1 v_{N^*}$  is  $O(\varepsilon)$ . For  $\bar{D}_1 v_{N^{**}-1}$  the coefficient is

$$\begin{aligned}
& -\frac{\varepsilon}{2}\phi'(\bar{D}_2 y_{N^{**}-1}) + \frac{3\varepsilon}{4}\phi''(\frac{1}{2}\bar{D}_2 y_{N^{**}-1} + \bar{D}_1 y_{N^{**}-1})[-\bar{D}_1 y_{N^{**}-1} + \bar{D}_1 y_{N^{**}}] \\
& + \frac{\varepsilon}{2}\phi'(\frac{1}{2}\bar{D}_2 y_{N^{**}-1} + \bar{D}_1 y_{N^{**}-1}). \tag{3.45}
\end{aligned}$$

We will use the Taylor expansion of  $\phi'(\bar{D}_2 y_{N^{**}-1})$  around  $(\frac{1}{2}\bar{D}_2 y_{N^{**}-1} + \bar{D}_1 y_{N^{**}})$  and substitute it into (3.45) as follows

$$\begin{aligned}
& -\frac{\varepsilon}{2}\phi'(\bar{D}_2 y_{N^{**}-1}) + \frac{3\varepsilon}{4}\phi''(\frac{1}{2}\bar{D}_2 y_{N^{**}-1} + \bar{D}_1 y_{N^{**}-1})[-\bar{D}_1 y_{N^{**}-1} + \bar{D}_1 y_{N^{**}}] \\
& + \frac{\varepsilon}{2}\phi'(\frac{1}{2}\bar{D}_2 y_{N^{**}-1} + \bar{D}_1 y_{N^{**}-1}) \\
& = -\frac{\varepsilon}{2}\phi'(\frac{1}{2}\bar{D}_2 y_{N^{**}-1} + \bar{D}_1 y_{N^{**}}) - \frac{\varepsilon}{4}\phi''(\frac{1}{2}\bar{D}_2 y_{N^{**}-1} + \bar{D}_1 y_{N^{**}})(\bar{D}_1 y_{N^{**}} - \bar{D}_1 y_{N^{**}-1}) \\
& - \frac{\varepsilon}{16}\phi'''(\frac{1}{2}\bar{D}_2 y_{N^{**}-1} + \bar{D}_1 y_{N^{**}})(\bar{D}_1 y_{N^{**}} - \bar{D}_1 y_{N^{**}-1})^2 \\
& + O\left(\left(\frac{\bar{D}_1 y_{N^{**}} - \bar{D}_1 y_{N^{**}-1}}{2}\right)^3\right) + \frac{\varepsilon}{2}\phi'(\frac{1}{2}\bar{D}_2 y_{N^{**}-1} + \bar{D}_1 y_{N^{**}}) \\
& + \frac{3\varepsilon}{4}\phi''(\frac{1}{2}\bar{D}_2 y_{N^{**}-1} + \bar{D}_1 y_{N^{**}})(-\bar{D}_1 y_{N^{**}-1} + \bar{D}_1 y_{N^{**}}) \\
& = \frac{1}{2}\varepsilon\phi''(\frac{1}{2}\bar{D}_2 y_{N^{**}-1} + \bar{D}_1 y_{N^{**}-1})(\bar{D}_1 y_{N^{**}} - \bar{D}_1 y_{N^{**}-1}) \\
& - \frac{\varepsilon}{16}\phi'''(\frac{1}{2}\bar{D}_2 y_{N^{**}-1} + \bar{D}_1 y_{N^{**}-1})(\bar{D}_1 y_{N^{**}} - \bar{D}_1 y_{N^{**}-1})^2 \\
& + O\left(\left(\frac{\bar{D}_1 y_{N^{**}} - \bar{D}_1 y_{N^{**}-1}}{2}\right)^3\right). \tag{3.46}
\end{aligned}$$



The order of  $\bar{D}_1 y_{N^{**}} - \bar{D}_1 y_{N^{**}-1}$  is  $O(\varepsilon)$  and hence the order of the coefficient of  $\bar{D}_1 v_{N^{**}-1}$  is  $O(\varepsilon)$ .

For  $\bar{D}_1 v_{N^{**}}$  the coefficient is

$$\begin{aligned} & \frac{\varepsilon}{2} \phi'(\bar{D}_2 y_{N^{**}-1}) + \frac{\varepsilon}{4} \phi''\left(\frac{1}{2} \bar{D}_2 y_{N^{**}-1} + \bar{D}_1 y_{N^{**}-1}\right) [-\bar{D}_1 y_{N^{**}-1} + \bar{D}_1 y_{N^{**}}] \\ & - \frac{\varepsilon}{2} \phi'\left(\frac{1}{2} \bar{D}_2 y_{N^{**}-1} + \bar{D}_1 y_{N^{**}-1}\right). \end{aligned} \quad (3.47)$$

We will use the Taylor expansion of  $\phi'(\bar{D}_2 y_{N^{**}-1})$  around  $(\frac{1}{2} \bar{D}_2 y_{N^{**}-1} + \bar{D}_1 y_{N^{**}})$  and substitute it into (3.47) as follows

$$\begin{aligned} & \frac{\varepsilon}{2} \phi'(\bar{D}_2 y_{N^{**}-1}) + \frac{\varepsilon}{4} \phi''\left(\frac{1}{2} \bar{D}_2 y_{N^{**}-1} + \bar{D}_1 y_{N^{**}-1}\right) [-\bar{D}_1 y_{N^{**}-1} + \bar{D}_1 y_{N^{**}}] \\ & - \frac{\varepsilon}{2} \phi'\left(\frac{1}{2} \bar{D}_2 y_{N^{**}-1} + \bar{D}_1 y_{N^{**}-1}\right) \\ & = \frac{\varepsilon}{2} \phi'\left(\frac{1}{2} \bar{D}_2 y_{N^{**}-1} + \bar{D}_1 y_{N^{**}}\right) + \frac{\varepsilon}{4} \phi''\left(\frac{1}{2} \bar{D}_2 y_{N^{**}-1} + \bar{D}_1 y_{N^{**}}\right) (\bar{D}_1 y_{N^{**}} - \bar{D}_1 y_{N^{**}-1}) \\ & + \frac{\varepsilon}{16} \phi'''\left(\frac{1}{2} \bar{D}_2 y_{N^{**}-1} + \bar{D}_1 y_{N^{**}}\right) (\bar{D}_1 y_{N^{**}} - \bar{D}_1 y_{N^{**}-1})^2 \\ & + O\left(\left(\frac{\bar{D}_1 y_{N^{**}} - \bar{D}_1 y_{N^{**}-1}}{2}\right)^3\right) - \frac{\varepsilon}{2} \phi'\left(\frac{1}{2} \bar{D}_2 y_{N^{**}-1}\right. \\ & \left. + \bar{D}_1 y_{N^{**}}\right) + \frac{\varepsilon}{4} \phi''\left(\frac{1}{2} \bar{D}_2 y_{N^{**}-1} + \bar{D}_1 y_{N^{**}}\right) (-\bar{D}_1 y_{N^{**}-1} + \bar{D}_1 y_{N^{**}}) \\ & = \frac{\varepsilon}{2} \phi''\left(\frac{1}{2} \bar{D}_2 y_{N^{**}-1} + \bar{D}_1 y_{N^{**}}\right) (\bar{D}_1 y_{N^{**}} - \bar{D}_1 y_{N^{**}-1}) \\ & + \frac{\varepsilon}{16} \phi'''\left(\frac{1}{2} \bar{D}_2 y_{N^{**}-1} + \bar{D}_1 y_{N^{**}}\right) (\bar{D}_1 y_{N^{**}} - \bar{D}_1 y_{N^{**}-1})^2 \\ & + O\left(\left(\frac{\bar{D}_1 y_{N^{**}} - \bar{D}_1 y_{N^{**}-1}}{2}\right)^3\right). \end{aligned} \quad (3.48)$$

The order of  $\bar{D}_1 y_{N^{**}} - \bar{D}_1 y_{N^{**}-1}$  is  $O(\varepsilon)$  and hence the order of the coefficient of  $\bar{D}_1 v_{N^{**}-1}$  is  $O(\varepsilon)$ . We are ready therefore to prove the main result of this chapter.

**Theorem 3.** (VARIATIONAL ERROR) *Let  $y$  be a smooth function; then, for any  $v \in \mathbb{V}_{\varepsilon, Q}$ , there exist a constant  $M_V = M_V(y, p)$ ,  $1 \leq p \leq \infty$ , independent of  $v$ , such that*

$$\left| \langle D\mathcal{E}_2^D\{y\}, v \rangle - \langle D\Phi^{CB}(y), v \rangle_\varepsilon \right| \leq M_V (\varepsilon^2 + \varepsilon^{2-1/p}) |v|_{W^{1,p}(\Omega)}.$$

*Proof.* Summarising what we have done so far, we see that

$$|\langle D\Phi_2^{CB}(y) - D\mathcal{E}_2^D(y), v \rangle_\varepsilon| \leq \varepsilon \sum_{\ell=1}^N |\alpha_\ell| |\bar{D}_1 v_\ell|, \quad (3.49)$$

where all but a finite number of  $\alpha_\ell$  satisfy  $|\alpha_\ell| \leq \gamma_1 \varepsilon^2$ ,  $\ell \in J$  and the remaining  $\alpha_\ell$  satisfy  $|\alpha_\ell| \leq \gamma_2 \varepsilon$ ,  $\ell \in J^C$ , where  $|J^C| \leq s$ , with  $s$  independent of  $N$ . We then have

$$(1/p + 1/q = 1)$$

$$\begin{aligned}
|\langle D\Phi_2^{CB}(y) - D\mathcal{E}_2^D(y), v \rangle_\varepsilon| &\leq \left( \varepsilon \sum_{\ell=1}^N |\alpha_\ell|^q \right)^{1/q} \left( \varepsilon \sum_{\ell=1}^N |\bar{D}_1 v_\ell|^p \right)^{1/p} \\
&= \left( \varepsilon \sum_{\ell \in J} |\alpha_\ell|^q + \varepsilon \sum_{\ell \in J^C} |\alpha_\ell|^q \right)^{1/q} \left( \varepsilon \sum_{\ell} |\bar{D}_1 v_\ell|^p \right)^{1/p} \\
&= \left( \varepsilon \sum_{\ell \in J} |\alpha_\ell|^q + \varepsilon \sum_{\ell \in J^C} |\alpha_\ell|^q \right)^{1/q} |v|_{W^{1,p}(\Omega)}
\end{aligned} \tag{3.50}$$

where in the last equality we have used that  $v \in \mathbb{V}_{\varepsilon,Q}$ . Now

$$\begin{aligned}
\left( \varepsilon \sum_{\ell \in J} |\alpha_\ell|^q + \varepsilon \sum_{\ell \in J^C} |\alpha_\ell|^q \right)^{1/q} &\leq \left( \varepsilon \sum_{\ell \in J} \gamma_1^q \varepsilon^{2q} + s \varepsilon \gamma_2^q \varepsilon^q \right)^{1/q} \\
&\leq \left( |\Omega| \gamma_1^q \varepsilon^{2q} + s \gamma_2^q \varepsilon^{q+1} \right)^{1/q} \\
&\leq C(\varepsilon^2 + \varepsilon^{(q+1)/q})
\end{aligned} \tag{3.51}$$

and the result follows by observing that  $(q+1)/q = 2 - 1/p$ .  $\square$

## 3.4 Numerical Simulations

For both the atomistic model and for the discontinuous bond volume based coupling method the sequential least squares programming optimizer function (SLSQP) was implemented in the Python programming language. This algorithm starts with an initial estimate and it finds the local minimum of the real valued scalar function which has several variables. The reason we chose this method was in order to be able to include constraints so that the atoms do not cross over each other which was observed when applying the Newton method and the conjugate gradient method.

### 3.4.1 Numerical Results

In the simulations, 100 atoms were considered and the first interface was set to  $N^* = 40$ , the 40th atom and the second interface was set to  $N^{**} = 60$ , the 60th atom. The initial condition was  $y_\ell = F\varepsilon\ell$  for  $\ell = 1, \dots, 100$ , the deformation gradient  $F = 1$  and the interatomic distance  $\varepsilon = 0.01$ . The Lennard-Jones potential and the Morse potential, already mentioned in Chapter 1, were used as the potential energy function. By setting the parameter  $a = 6/r_e$  in the Morse potential [14] the Lennard Jones potential and the Morse potential have a very similar shape and so can be compared more easily. In the figures below we will display the results of the fully atomistic method and the discontinuous bond volume based coupling method for the Morse potential and the Lennard-Jones potential. The external forces that are applied are all equivalent in magnitude and the energy will also be given. We will consider four cases for the external forces

- Case 1: External forces on the interfaces ( $f(40) > 0, f(60) < 0$ )
- Case 2: Opposite external forces between the interfaces ( $f(42) > 0, f(56) < 0$ )

- Case 3: Opposite external forces outside the interfaces ( $f(10) > 0, f(80) < 0$ )
- Case 4: One constant external force for all the atoms up to  $N/2$  and the opposite constant external force for the atoms from  $N/2$  up to  $N$ ,

$$f(a, b) = \begin{cases} f(i) > 0 & \text{for } i = 1, \dots, \frac{N}{2} - 1 \\ f(i) < 0 & \text{for } i = \frac{N}{2}, \dots, N. \end{cases}$$

In case 1 the external forces are on the interfaces, a positive force is applied on the first interface and a negative force on the second interface. The atoms between the two interfaces are pushed against each other and so the distance between the atoms decreases whereas the atoms in both atomistic regions are pulled against each other and so the atoms have a greater distance between each other. This is displayed in Figures 3.1(b),(d), (f) and (h) where the strain is negative between the two interfaces because the difference between the displacement of the solution and  $\varepsilon$  (the initial distance between the atoms) is negative. The solutions for the minimisation problem for case 1 are displayed in Figures 3.1(a), (c), (e) and (g).

In case 2 the external forces are applied between the interfaces, there is a positive force on atom 42 and a negative force on atom 56. The atoms between atoms 42 and 56 are pushed against each other and so the distance between the atoms decreases whereas the rest of the atoms are pulled against each other and so the atoms have a greater distance between each other. This is displayed in Figures 3.2(b),(d), (f) and (h) where the strain is negative between atoms 42 and 56 because the difference between the displacement of the solution and  $\varepsilon$  (the initial distance between the atoms) is negative. The solutions for the minimisation problem for case 2 are displayed in Figures 3.2(a), (c), (e) and (g).

In case 3 the external forces are outside the interfaces, there is a positive force on the 10th atom and a negative force on the 80th atom. The atoms between the 10th and the 80th atom are pushed against each other and so the distance between the atoms decreases whereas the rest of the atoms are pulled against each other and so the atoms have a greater distance between each other. This is displayed in Figures 3.3(b),(d), (f) and (h) where the strain is negative between the 10th atom and the 80th atom because the difference between the displacement of the solution and  $\varepsilon$  (the initial distance between the atoms) is negative. The solutions for the minimisation problem for case 3 are displayed in Figures 3.3(a), (c), (e) and (g).

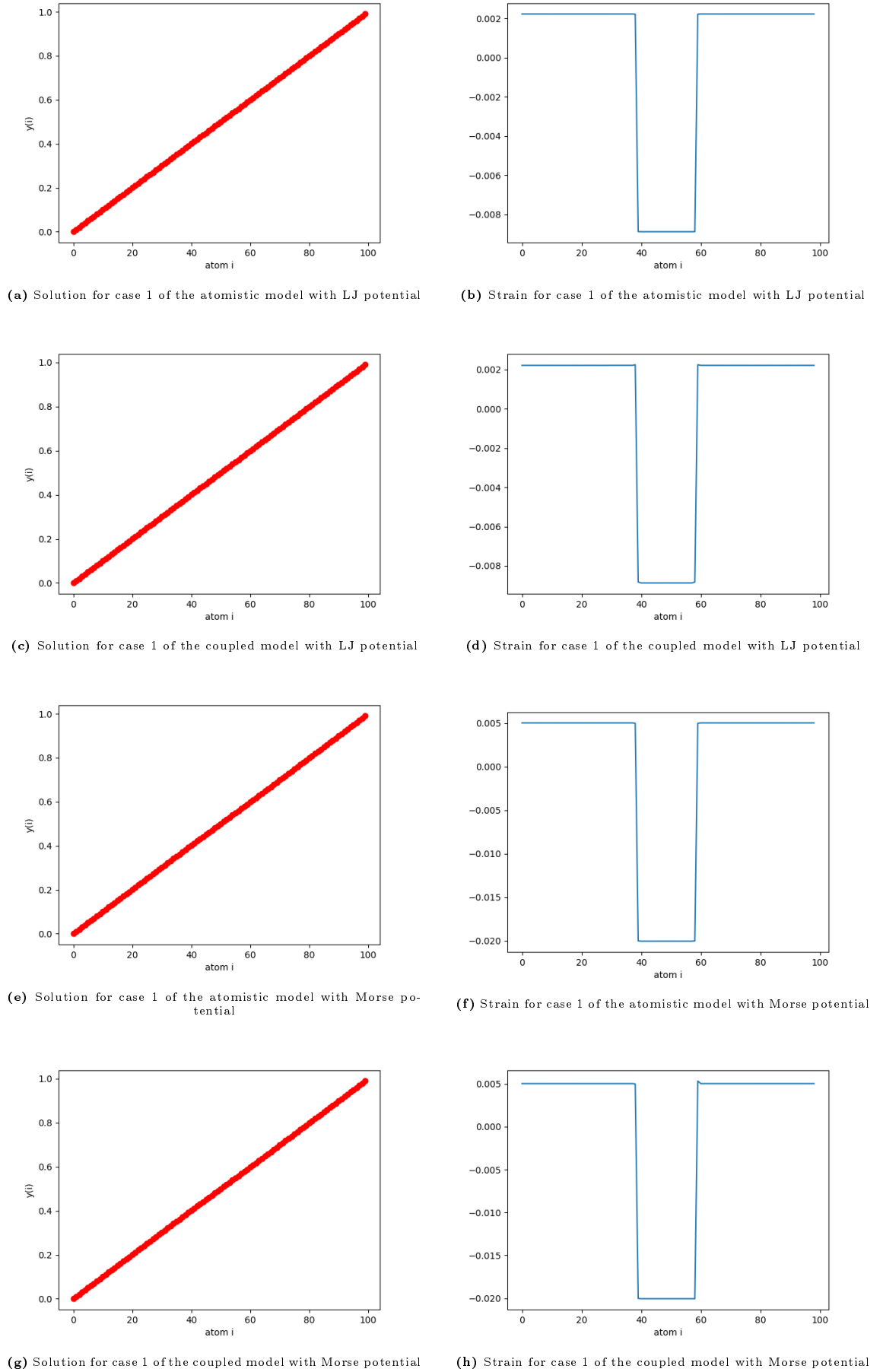
In case 4 a constant positive external force is applied on each of the first  $N/2$  atoms and a constant negative force on each of the atoms from atoms  $N/2$  to  $N$ . The atoms closer to atom  $N/2$  have a greater strain because they are closer to the atom that is in between two opposite forces. This is displayed in Figures 3.4(b),(d), (f) and (h) where the strain is negative for all the atoms. The solutions for the minimisation problem for case 4 are displayed in Figures 3.4(a), (c), (e) and (g).

The errors, for each case, between the atomistic model and the coupled model for both the Lennard-Jones potential and the Morse potential are displayed in Figure

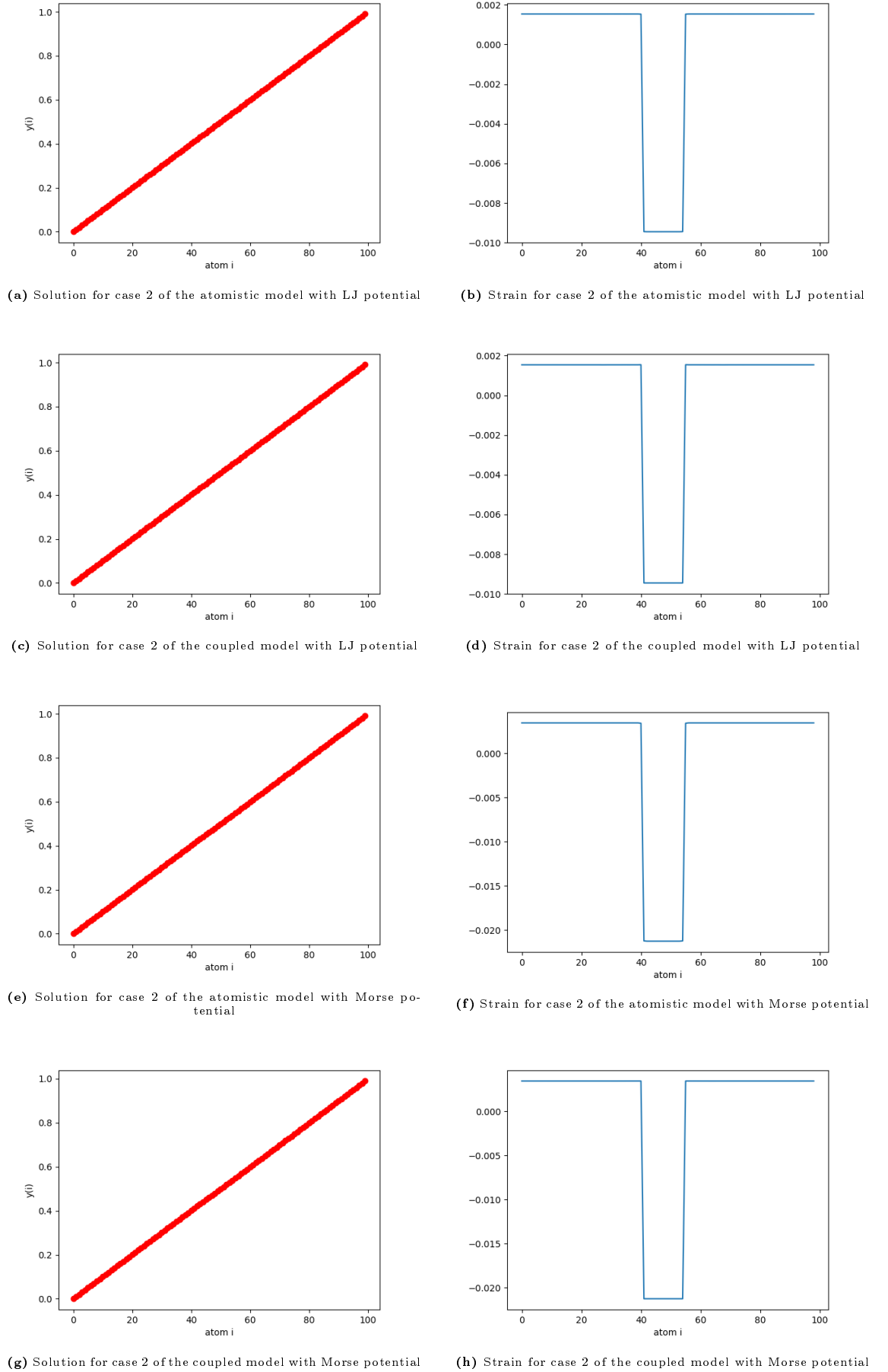
3.5 and in Table 3.1. From both the diagrams and the table it can be deduced that the errors are of a satisfactory order.

	Error for Lennard Jones potential	Error for Morse potential
Case1	3.62799E-07	1.01613E-06
Case2	4.51292E-08	7.04004E-08
Case3	6.48871E-08	5.76108E-08
Case4	7.67919E-08	2.6196E-07

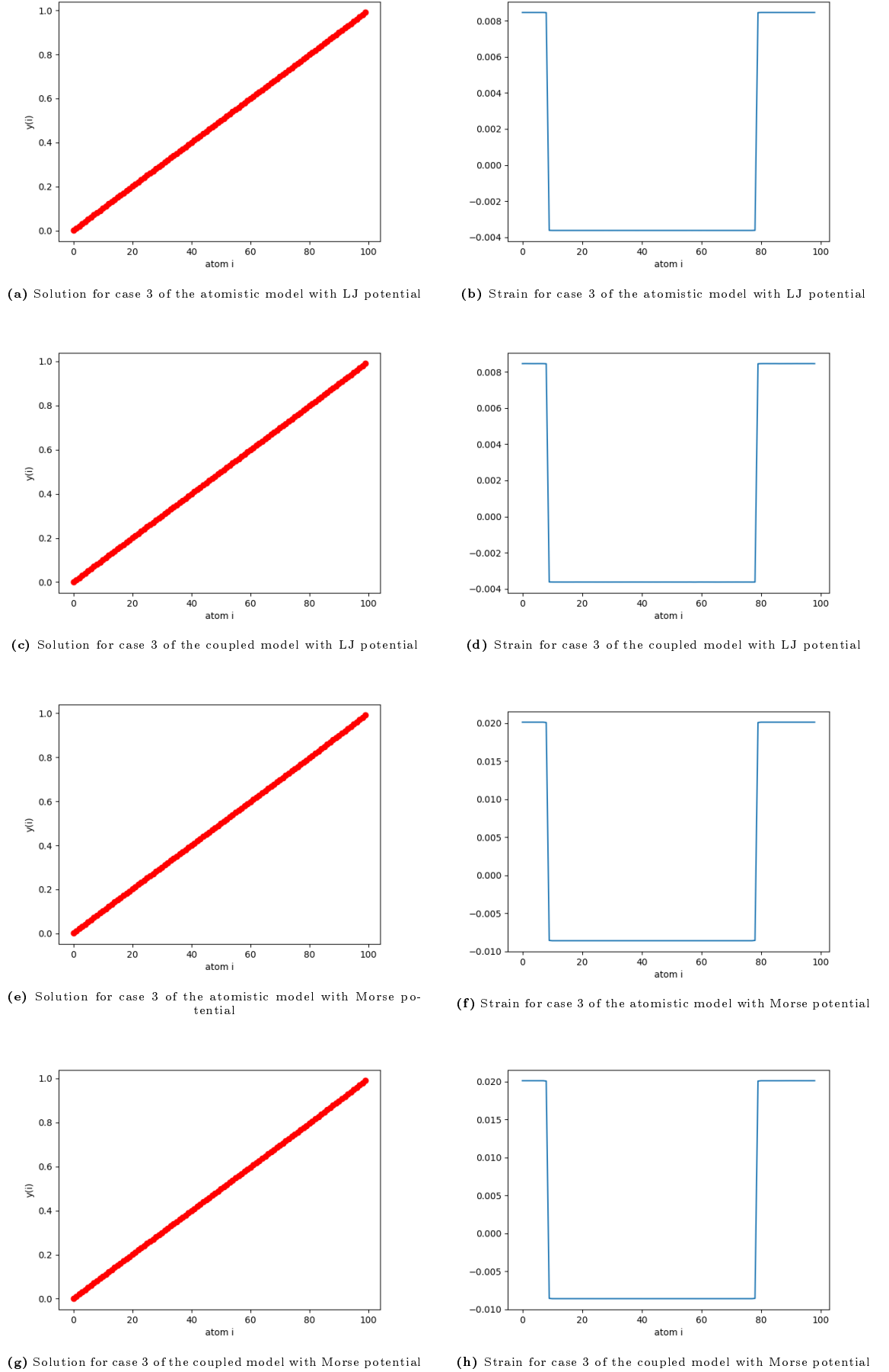
**Table 3.1:** Table of errors for Lennard Jones potential and for Morse potential



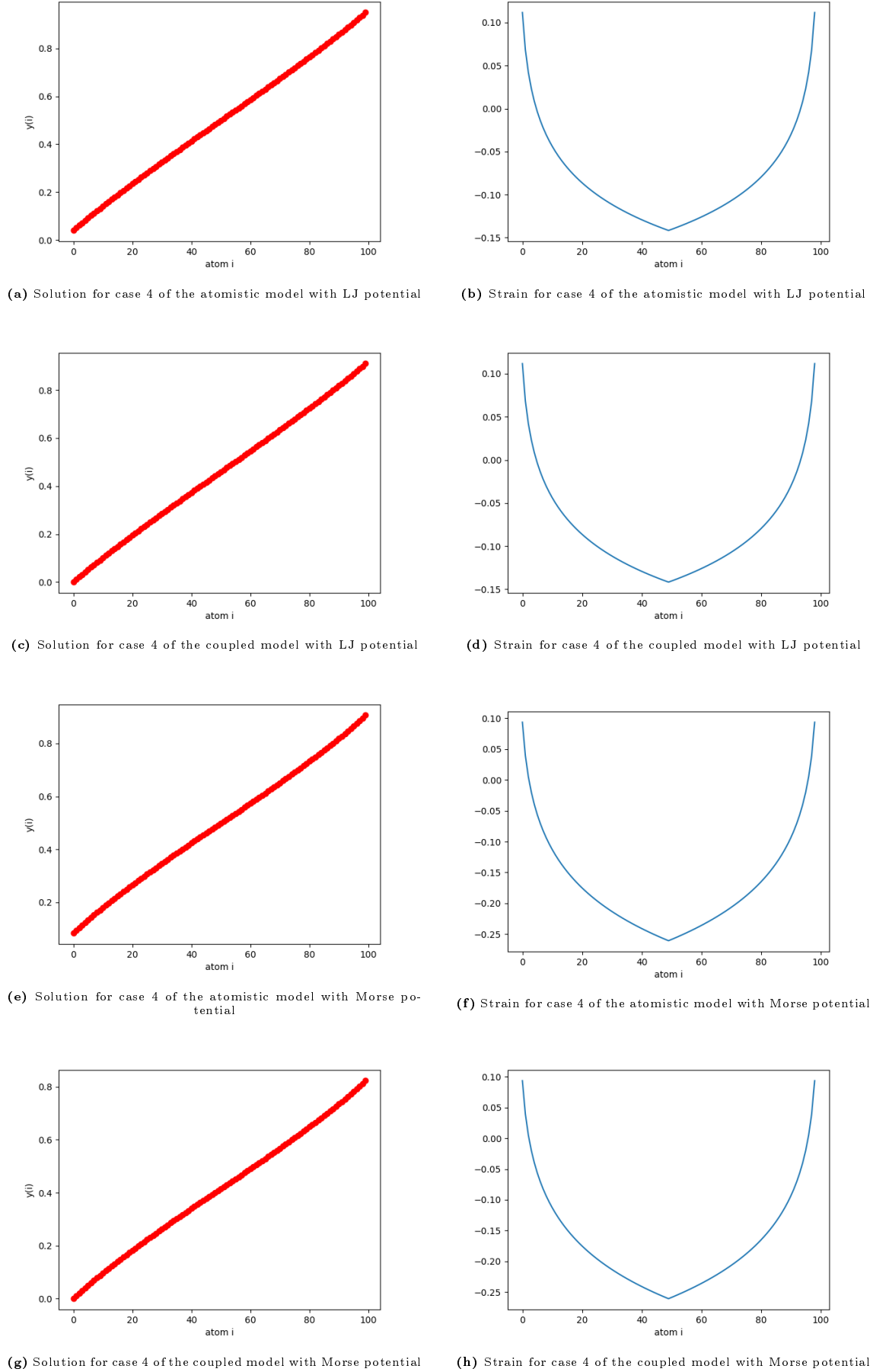
**Figure 3.1:** Casel: External forces on the interfaces ( $f(40) > 0, f(60) < 0$ ) for Lennard-Jones potential and for Morse potential



**Figure 3.2:** Opposite external forces between the interfaces ( $f(42) > 0, f(56) < 0$ ) for Lennard-Jones potential and for Morse potential

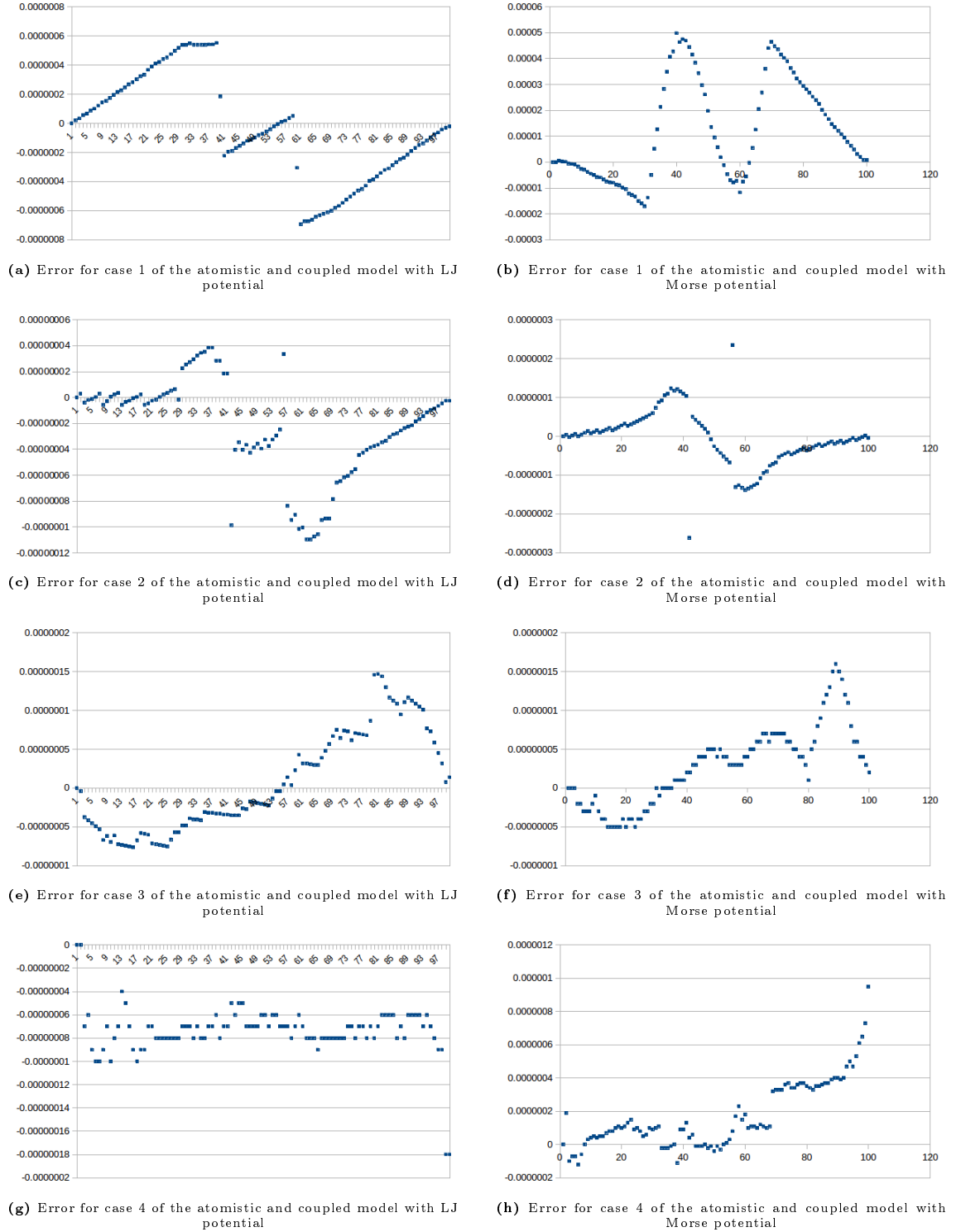


**Figure 3.3:** Opposite external forces outside the interfaces ( $f(10) > 0, f(80) < 0$ ) for Lennard-Jones potential and for Morse potential



**Figure 3.4:** One constant external force for all the atoms up to  $N/2$  and the opposite constant external force for the atoms from  $N/2$  up to  $N$ , for the Lennard-Jones potential and for Morse potential





**Figure 3.5:** The error for each of the four cases we considered of the atomistic and coupled model with Lennard Jones potential (a),(c),(e),(g) and Morse potentials (b),(d),(f),(h).

# Chapter 4

## Energy Consistency Analysis in 2D

### 4.1 Chapter Overview

In this chapter we introduce a new two dimensional discontinuous coupled method and we analyse its energy consistency. Section 4.2 contains the notation and some definitions that will be used in the chapter. In Section 4.3 we show that the model

$$E_{\Omega_*,\eta}^a\{y\} = \varepsilon^2 \sum_{K \subset \Omega_*} \phi(\bar{\nabla} y \eta),$$

is a second order approximation of the continuum Cauchy-Born model. For technical reasons we use this atomistic Cauchy-Born model as a tool and in particular as the model in the continuum region. In Section 4.4 we define the total coupling energy (4.19)

$$\mathcal{E}_\eta^D\{y\} = E_{\Omega_a,\eta}^a\{y\} + E_{\Gamma,\eta}^D\{y\} + E_{\Omega_*,\eta}^{a,CB}\{y\},$$

where the atomistic energy and the energy on the interface are defined explicitly. Note that although the interface term  $E_{\Gamma,\eta}^D\{y\}$  is defined and analysed in this chapter, its design is motivated in the next chapter. This is because, as noted earlier, energy consistency analysis alone cannot detect force inconsistencies. We show that the method motivated by the analysis of first variations in Chapter 5 is indeed consistent at the energy and at first variations level. In Section 4.5 we compute the difference between the atomistic Cauchy-Born energy over the whole domain and coupled energy as in (4.28). We focus first on the difference between the atomistic Cauchy-Born energy and the atomistic energy from the coupled energy. In order to be able to subtract the atomistic energies from the atomistic Cauchy-Born energy, we need to convert the atomistic energies into a similar form as the atomistic Cauchy-Born energy. For the atomistic energy we create symmetries of the form

$$\phi(\bar{D}_\eta y(x_{\ell_1}, x_{\ell_2})) + \phi(\bar{D}_\eta y(x_{\ell_1+1}, x_{\ell_2})) + \phi(\bar{D}_\eta y(x_{\ell_1}, x_{\ell_2+1})) + \phi(\bar{D}_\eta y(x_{\ell_1+1}, x_{\ell_2+1}))$$

so that later on when we subtract it from the atomistic Cauchy-Born energy we can apply

$$\left| \frac{1}{4} \left[ \phi(\bar{D}_\eta y(x_{\ell_1}, x_{\ell_2})) + \phi(\bar{D}_\eta y(x_{\ell_1+1}, x_{\ell_2})) + \phi(\bar{D}_\eta y(x_{\ell_1}, x_{\ell_2+1})) + \phi(\bar{D}_\eta y(x_{\ell_1+1}, x_{\ell_2+1})) \right] - \phi \left( \nabla y(m_{K_{e_1+e_2}}) \binom{2}{2} \right) \right| \leq c\varepsilon^2$$

which is a combination of Lemmas 21 and 22 in Section 4.5.1. Then we add each of the atomistic energies  $E_{\Omega_{a_1}}, E_{\Omega_{a_2}}, E_{\Omega_{a_3}}$  and  $E_{\Omega_{a_4}}$  and gather the terms in a way where we have terms corresponding to the inner cells of the whole atomistic region,  $A_{inner}$ , terms corresponding to the cells on the external boundary of the atomistic region  $A_{ext,B}$  and terms corresponding to the interfaces  $A_\Gamma$

$$\begin{aligned} E_{\Omega_{a,\eta}}^a\{y\} &= E_{\Omega_{a_1,\eta}}^a\{y\} + E_{\Omega_{a_2,\eta}}^a\{y\} + E_{\Omega_{a_3,\eta}}^a\{y\} + E_{\Omega_{a_4,\eta}}^a\{y\} \\ &= A_{inner} + A_{ext,B} + A_\Gamma. \end{aligned}$$

The energy on the interfaces is defined in Section 4.6. As mentioned, the introduction of the interface terms is motivated by the analysis in Chapter 5. The new interfacial energy is a variation of the one discussed in Chapter 1 that was introduced in [19]. We summarise the analysis in Lemma 18

$$\begin{aligned} \Phi_\eta^{CB}(y) - \mathcal{E}_\eta^D(y) &= \varepsilon^2 \sum_{K \subset T_{\Omega_{a_1}} \cup T_{\Omega_{a_2}} \cup T_{\Omega_{a_3}} \cup T_{\Omega_{a_4}}} \phi(\nabla y(m_K)\eta) - A_{inner} - A_{ext,B} - A_\Gamma \\ &\quad - E_{\Gamma,\eta}(y) + \mathcal{O}(\varepsilon^2) \\ &=: \Theta_B - A_\Gamma - E_{\Gamma,\eta}(y) + \mathcal{O}(\varepsilon^2). \end{aligned}$$

In Section 4.5.1 we state Lemmas 19- 22 which when applied to  $\Theta_B$  results in (4.71). In Section 4.6 we define the energy on the interfaces which have the form they do due to the analysis in Chapter 5. In Section 4.6.1 we continue the calculations of (4.40) in (4.80) but now we also consider the energy on the interaces  $E_{\Gamma,\eta}(y)$ . By rearranging the terms and by applying Lemma 22. The terms that remain are in (4.92). We check the order of these terms by using Taylor expansion and we observe that they are of order  $O(\varepsilon)$ . Finally, we prove in Theorem 5 on page 98 that the coupled energy for  $\eta = 2$  is a second order approximation to the atomistic Cauchy-Born energy. This holds despite the fact that terms around the interface are locally only  $\mathcal{O}(\varepsilon)$ . This is in contrast to the one dimensional case, see the proof of Theorem 5 for details. The results of this chapter apply to the energy in [19] as well with appropriate but straightforward modifications.

## 4.2 Definitions and Notation

We recall from Chapter 1 the two dimensional lattice settings. Let  $\mathcal{L}_{entire} = \mathbb{Z}^2$  be a two-dimensional lattice that is generated from two linearly independent vectors  $e_1, e_2$  of  $\mathbb{R}^2$ . Consider discrete periodic functions of  $\mathcal{L}_{entire}$  defined over a ‘periodic domain’  $\mathcal{L}$ . Let

$$\mathcal{L} = \{\ell = (\ell_1, \ell_2) \in [1, N] \times [1, N], \quad N \in \mathbb{N}\}.$$

The configuration of the atoms before deformation is defined as

$$\Omega_{discr} = \{x_\ell = (x_{\ell_1}, x_{\ell_2}) = (\varepsilon\ell_1, \varepsilon\ell_2), \quad \ell_1 \in [1, N], \quad \ell_2 \in [1, N]\}.$$

Let  $y : [1, N] \times [1, N] \rightarrow \mathbb{R}^2$  be the atomistic deformation such that, for  $\ell \in \mathcal{L}$ ,

$$y_\ell = y(x_\ell) = y(x_{\ell_1}, x_{\ell_2}) = \begin{bmatrix} y^1(x_{\ell_1}, x_{\ell_2}) \\ y^2(x_{\ell_1}, x_{\ell_2}) \end{bmatrix} \quad (4.1)$$

with  $y_\ell = Fx_\ell + v_\ell$ , where  $v_\ell = v(x_{\ell_1}, x_{\ell_2})$  is periodic with respect to  $\mathcal{L}$  and  $F$  is a constant  $2 \times 2$  matrix with  $\det(F) > 0$ . The function spaces for  $y$  and  $v$  are denoted by  $\mathcal{X}$  and  $\mathcal{V}$ .

Let us denote the finite element mesh of  $\Omega$  consisting of atomistic cells as

$$T = \{K \subset \Omega : K = (x_{\ell_1}, x_{\ell_1+1}) \times (x_{\ell_2}, x_{\ell_2+1}), \quad x_\ell = (x_{\ell_1}, x_{\ell_2}) \in \Omega_{discr}\}, \quad (4.2)$$

and let  $m_K$  be the barycenter of  $K$ .

### 4.3 Continuum Cauchy-Born Potential Energy

We will state the following result which will be used in the forthcoming lemma, Lemma 17, see [21], which is a variation of Bramble-Hilbert lemma [6]

**Lemma 16** (Bramble Hilbert). *Let  $\mathcal{O}$  be a bounded open set in  $\mathbb{R}^d$  and suppose that  $1 \leq p \leq \infty$  and  $s \geq 0$ . Suppose further that  $\zeta$  is a linear functional on a linear subspace  $\mathbb{H}$  of  $W^{s,p}(\mathcal{O})$  with the following property:*

$$\exists C_0 > 0 \quad \forall w \in \mathbb{H} : |\zeta(w)| \leq C_0 \|w\|_{W^{s,p}(\mathcal{O})}.$$

*Then, for any  $w \in \mathbb{H}$  and any set  $\mathbb{S} \subset \text{Ker}(\zeta)$  we have that*

$$|\zeta(w)| \leq C_0 \inf \|w - \phi\|_{W^{s,p}(\mathcal{O})}.$$

*If in addition, there exists a positive constant  $C_1$ , independent of  $\text{diam}(\mathcal{O})$ , and a real number  $t > s$  such that*

$$\inf \|w - \phi\|_{W^{s,p}(\mathcal{O})} \leq C_1 (\text{diam}(\mathcal{O}))^{t-s} |w|_{W^{t,p}(\mathcal{O})},$$

*where  $|\cdot|_{W^{t,p}(\mathcal{O})}$  is the standard semi-norm on  $W^{t,p}(\mathcal{O})$ , then*

$$|\zeta(w)| \leq C_0 C_1 (\text{diam}(\mathcal{O}))^{t-s} |w|_{W^{t,p}(\mathcal{O})}.$$

The following lemma is needed in Theorem 3 later on.

**Lemma 17.** *Let*

$$I_2 = \sum_{K \in T} \int_K \left[ W_{CB}(\nabla y(x)) - W_{CB}(\nabla y(m_K)) \right] dx. \quad (4.3)$$

*Then there exists a constant  $C(y)$  independent of  $\varepsilon$  such that*

$$|I_2| \leq C(y) \varepsilon^2. \quad (4.4)$$

*Proof.* We denote by  $\zeta$  the linear functional

$$\zeta(w) := \frac{1}{|K|} \int_K \left\{ w(x_1, x_2) - w(m_K) \right\} dx_1 dx_2, \quad (4.5)$$

and observe that

$$\zeta(\phi) = 0, \quad \forall \phi \in \mathbb{Q}_1(K), \quad (4.6)$$

where  $\mathbb{Q}_1(K)$  denotes the set of all bilinear functions on  $K$ . For  $w \in \mathbb{Q}_1(K)$ , we have

$$\begin{aligned} w(x_1, x_2) &= c_0 + c_1 x_1 + c_2 x_2 + c_3 x_1 x_2 \\ &= (\gamma_0 + \gamma_1 x_1)(\delta_0 + \delta_1 x_2) \\ &= \beta_1(x_1)\beta_2(x_2). \end{aligned} \quad (4.7)$$

Let  $x_1^m$  be the middle point between  $x_{\ell_1}$  and  $x_{\ell_1+1}$  and  $x_2^m$  be the middle point between  $x_{\ell_2}$  and  $x_{\ell_2+1}$ , then

$$\begin{aligned} \int_K w(x_1, x_2) dx_1 dx_2 &= \int_K \beta_1(x_1)\beta_2(x_2) dx_1 dx_2 \\ &= \int_{x_{\ell_2}}^{x_{\ell_2+1}} \beta_2(x_2) \left( \int_{x_{\ell_1}}^{x_{\ell_1+1}} \beta_1(x_1) dx_1 \right) dx_2 \\ &= \int_{x_{\ell_2}}^{x_{\ell_2+1}} \beta_2(x_2) \varepsilon \beta_1(x_1^m) dx_2 \quad (\text{due to linearity of } \beta_1) \\ &= \varepsilon \beta_1(x_1^m) \int_{x_{\ell_2}}^{x_{\ell_2+1}} \beta_2(x_2) dx_2 \quad (\text{due to linearity of } \beta_2) \\ &= \varepsilon^2 \beta_1(x_1^m) \beta_2(x_2^m) := \varepsilon^2 w(m_K). \end{aligned} \quad (4.8)$$

So, we clearly have  $\zeta(w) = 0$ ,  $\forall w \in \mathbb{Q}_1(K)$ . In view of applying Lemma 16 we show that

$$|\zeta(v)| \leq 2\|v\|_{L^\infty(K)}, \quad \text{for every } v \in C(\bar{K}). \quad (4.9)$$

So,

$$\begin{aligned} |\zeta(v)| &= \frac{1}{|K|} \left| \int_K \{v(x_1, x_2) - v(m_K)\} dx_1 dx_2 \right| \\ &\leq \frac{1}{|K|} \int_K |v(x_1, x_2)| dx_1 dx_2 + \frac{1}{|K|} \int_K |v(m_K)| dx_1 dx_2 \\ &= 2\|v\|_{L^\infty(\Omega)}, \end{aligned} \quad (4.10)$$

where

$$\|v\|_{L^\infty(\Omega)} = \text{ess sup} |v(x_1, x_2)|. \quad (4.11)$$

Hence, for a linear functional  $\zeta$ , which is zero on  $\mathbb{S} = \mathbb{Q}_1(K)$  and that satisfies  $|\zeta(w)| \leq C_0 \|w\|_{L^\infty(K)}$  for all  $w \in \mathbb{H} = C(\bar{K})$  we can apply Lemma 16 with  $p = \infty$ ,  $s = 0$  and  $t = 2$  so that

$$|\zeta(w)| \leq C_0 C_1 \varepsilon^2 \sum_{\alpha=1}^d \|\partial_\alpha^2 w\|_{L^\infty(K)}, \quad \forall w \in W^{2,\infty}(K). \quad (4.12)$$

Therefore, with  $w(\cdot) = W_{CB}(\nabla y(\cdot))$ ,

$$\begin{aligned} & \left| \sum_{K \in T} \left[ \int_K W_{CB}(\nabla y(x)) dx - |K| W_{CB}(\nabla y(m_K)) \right] \right| \\ & \leq C\varepsilon^2 \sum_{K \in T} |K| \sum_{\alpha=1}^2 \|\partial_\alpha^2 W_{CB}(\nabla y(\cdot))\|_{L^\infty(K)} \\ & \leq C\varepsilon^2 |\Omega| \|\partial_\alpha^2 W_{CB}(\nabla y(\cdot))\|_{L^\infty(\Omega)}. \end{aligned} \quad (4.13)$$

□

Now, we will introduce the energy consistency theorem comparing the energies of the atomistic and the Cauchy-Born models.

**Theorem 4.** (*Energy Consistency*) *Let  $y$  be a smooth function, then there exists a constant  $M_E = M_E(y)$ , such that*

$$|\Phi_2^{CB}(y) - \Phi_2^a(y)| \leq M_E \varepsilon^2. \quad (4.14)$$

*Proof.* The proof is given in [21].

□

## 4.4 Atomistic to Continuum Coupled Energy

The domain of the two dimensional problem is displayed in Figure 4.1. The domains  $\Omega_{a_1}, \Omega_{a_2}, \Omega_{a_3}$  and  $\Omega_{a_4}$  are the atomistic domains,  $\Gamma_1, \Gamma_2, \Gamma_3$  and  $\Gamma_4$  compose the interface  $\Gamma$  and the atomistic Cauchy-Born domain is  $\Omega_*$ . Specifically, the atomistic and atomistic Cauchy-Born domains are given in Section 4.5, (4.25-4.27). It is noted that the interfaces have no thickness.

Recall the coupled energy introduced in Chapter 1, (1.40) which is mentioned again in Chapter 5, (5.32)

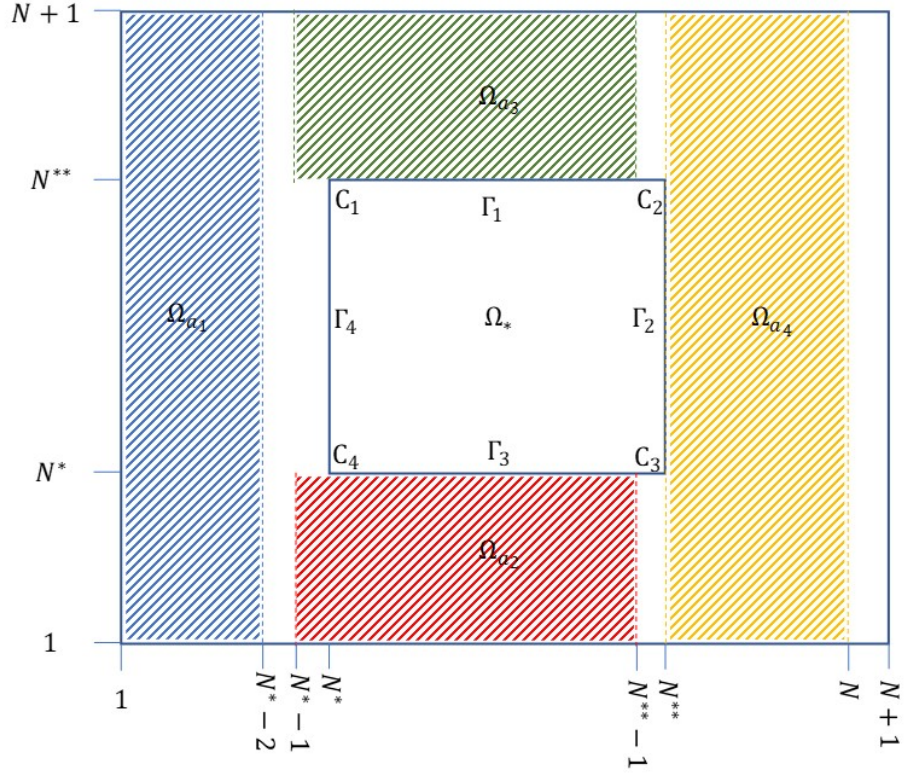
$$\begin{aligned} E_{\Gamma, \eta}^D \{y\} &= \sum_{\substack{\ell \in \mathcal{L} \\ B_{\ell, \eta} \in B_\Gamma}} \frac{1}{|\eta_1 \eta_2|} \left[ \int_{B_{\ell, \eta}} \chi_{\Omega_a} \phi(\nabla y^{\ell, \eta} \eta) dx - \int_{B_{\ell, \eta} \cap \Gamma} \phi'(\{\nabla y^{\ell, \eta} \eta\}) \cdot \llbracket y^{\ell, \eta} \eta \rrbracket dS \right] \\ &=: E_1 + E_2. \end{aligned} \quad (4.15)$$

where  $\eta = (\eta_1, \eta_2)$  and  $B_{\ell, \eta}$  is a bond volume that is an open quadrilateral that has vertices  $x_\ell, x_{\ell+\eta_1 e_1}, x_{\ell+\eta_2 e_2}, x_{\ell+\eta}$ . The bond volumes that intersect the interfaces are given in Figures 4.4 and 4.5. The coupled energy we will work with will be a modification of this energy. The first modification is that in the first term  $E_1$  we replace  $\nabla y^{\ell, \eta} \eta$  with  $\overline{D}_\eta y_\ell$  which becomes

$$\sum_{\substack{\ell \in \mathcal{L} \\ B_{\ell, \eta} \in B_\Gamma}} \frac{1}{|\eta_1 \eta_2|} \int_{B_{\ell, \eta}} \chi_{\Omega_a} \phi(\overline{D}_\eta y_\ell) dx. \quad (4.16)$$

For example, the energy on interface  $\Gamma_1$  corresponding to term  $E_1$  is (5.33)

$$E_{1, \Gamma_1} \{y\} = \sum_{\ell_1 = N^*}^{N^{**}-2} \frac{1}{4} \int_{B_{(\ell_1, N^{**}-1), \eta}} \chi_{\Omega_a} \phi(\overline{D}_\eta y_\ell) dx. \quad (4.17)$$



**Figure 4.1:** Displaying  $\Omega_{a1}, \Omega_{a2}, \Omega_{a3}, \Omega_{a4}$  and the interfaces  $\Gamma_1, \Gamma_2, \Gamma_3, \Gamma_4$

The second modification is that the second term  $E_2$  takes a different form. The form it takes is a result of the calculations in Chapter 5. Specifically, when calculating the difference between the first variation of the coupled energy and the first variation of the atomistic Cauchy-Born energy in Chapter 5 the aim was to obtain an error of a satisfactory order. In the analysis of the difference of these two first variations there were certain terms, (5.62) - (5.69) that had to be removed in order to retain consistency of the first variation. The way this was done was to create an  $E_2$  term whose first variation would compensate with the terms that had to be removed. These  $E_2$  terms are given in equations (4.72)- (4.79). For example, the energy on interface  $\Gamma_1$  in the  $e_2$  direction corresponding to term  $E_2$  (4.72) is

$$\begin{aligned}
 E_{2,\Gamma_1}\{y\} = & -\frac{\varepsilon^2}{4} \sum_{\ell_1=N^*}^{N^{**}-1} \nabla_{\zeta} \phi(\bar{D}_{\eta} y(x_{\ell_1}, x_{N^{**}-1})) [\bar{D}_{e_2} y(x_{\ell_1}, x_{N^{**}-1}) - \bar{D}_{e_2} y(x_{\ell_1}, x_{N^{**}})] \\
 & -\frac{\varepsilon^2}{4} \sum_{\ell_1=N^*}^{N^{**}-1} \nabla_{\zeta} \phi(\bar{D}_{\eta} y(x_{\ell_1-2}, x_{N^{**}-1})) [\bar{D}_{e_2} y(x_{\ell_1}, x_{N^{**}-1}) - \bar{D}_{e_2} y(x_{\ell_1}, x_{N^{**}})].
 \end{aligned}
 \tag{4.18}$$

The results of this chapter apply to both, the energy defined in Chapter 1, and the new coupled energy. However, we provide detailed analysis only for the new coupled energy. Similar arguments can be used when analysing the energy defined in Chapter 1. We define the total coupling energy as

$$\mathcal{E}_{\eta}^D\{y\} = E_{\Omega_a, \eta}^a\{y\} + E_{\Gamma, \eta}^D\{y\} + E_{\Omega_*, \eta}^{a, CB}\{y\},
 \tag{4.19}$$

where

$$E_{\Omega_{a,\eta}}^a\{y\} = E_{\Omega_{a_1,\eta}}^a\{y\} + E_{\Omega_{a_2,\eta}}^a\{y\} + E_{\Omega_{a_3,\eta}}^a\{y\} + E_{\Omega_{a_4,\eta}}^a\{y\}, \quad (4.20)$$

and the interfacial energy will be defined as,

$$\begin{aligned} E_{\Gamma,\eta}^D\{y\} = & E_{\Gamma_1}\{y\} + E_{\Gamma_2}\{y\} + E_{\Gamma_3}\{y\} + E_{\Gamma_4}\{y\} \\ & + E_{C_1}\{y\} + E_{C_2}\{y\} + E_{C_3}\{y\} + E_{C_4}\{y\}. \end{aligned} \quad (4.21)$$

The components of the energy  $E_{\Gamma,\eta}^D(y)$  will be given in Section 4.6. We will assume for the rest of the chapter that  $\eta = (2, 2)$ . For fixed  $\eta = (2, 2)$ ,

$$\begin{aligned} E_{\Omega_{a_1,\eta}}^a\{y\} &= \varepsilon^2 \sum_{\ell_1=1}^{N^*-2} \sum_{\ell_2=1}^N \phi(\overline{D}_\eta y(x_{\ell_1}, x_{\ell_2})), \\ E_{\Omega_{a_2,\eta}}^a\{y\} &= \varepsilon^2 \sum_{\ell_1=N^*-1}^{N^{**}-1} \sum_{\ell_2=1}^{N^*-2} \phi(\overline{D}_\eta y(x_{\ell_1}, x_{\ell_2})), \\ E_{\Omega_{a_3,\eta}}^a\{y\} &= \varepsilon^2 \sum_{\ell_1=N^*-1}^{N^{**}-1} \sum_{\ell_2=N^{**}}^N \phi(\overline{D}_\eta y(x_{\ell_1}, x_{\ell_2})), \\ E_{\Omega_{a_4,\eta}}^a\{y\} &= \varepsilon^2 \sum_{\ell_1=N^{**}}^N \sum_{\ell_2=1}^N \phi(\overline{D}_\eta y(x_{\ell_1}, x_{\ell_2})), \end{aligned} \quad (4.22)$$

and

$$E_{\Omega_*,\eta}^a\{y\} = \varepsilon^2 \sum_{K \subset \Omega_*} \phi(\overline{\nabla} y \eta). \quad (4.23)$$

where the domains of the energies are displayed in Figure 4.1. Recall that Lemma 17 implies,

$$E_{\Omega_*,\eta}^a\{y\} = \varepsilon^2 \sum_{K \subset \Omega_*} \phi(\nabla y(m_K)\eta) + O(\varepsilon^2). \quad (4.24)$$

## 4.5 Comparison of Coupled Energy with Continuum Energy

Let us define the atomistic domains

$$\begin{aligned} T_{\Omega_{a_1}} &= \{[x_1, x_{N^*}] \times [x_1, x_{N+1}]\} \\ T_{\Omega_{a_2}} &= \{[x_{N^*}, x_{N^{**}}] \times [x_1, x_{N^*}]\} \\ T_{\Omega_{a_3}} &= \{[x_{N^*}, x_{N^{**}}] \times [x_{N^{**}}, x_{N+1}]\} \\ T_{\Omega_{a_4}} &= \{[x_{N^{**}}, x_{N+1}] \times [x_1, x_{N+1}]\}, \end{aligned} \quad (4.25)$$

the atomistic Cauchy-Born domain

$$T_{\Omega_*} = \{[x_{N^*}, x_{N^{**}}] \times [x_{N^*}, x_{N^{**}}]\}, \quad (4.26)$$



and,

$$\begin{aligned}
\Phi_\eta^{CB}(y) &= \varepsilon^2 \sum_{K \subset T_{\Omega_{a_1}}} \phi(\nabla y(m_K)\eta) + \varepsilon^2 \sum_{K \subset T_{\Omega_{a_2}}} \phi(\nabla y(m_K)\eta) + \varepsilon^2 \sum_{K \subset T_{\Omega_{a_3}}} \phi(\nabla y(m_K)\eta) \\
&\quad + \varepsilon^2 \sum_{K \subset T_{\Omega_{a_4}}} \phi(\nabla y(m_K)\eta) + \varepsilon^2 \sum_{K \subset T_{\Omega_*}} \phi(\nabla y(m_K)\eta) + O(\varepsilon^2) \\
&:= A_{CB} + B_{CB} + C_{CB} + D_{CB} + G_{CB} + O(\varepsilon^2).
\end{aligned} \tag{4.27}$$

Our starting point is the error equation

$$\begin{aligned}
\Phi_\eta^{CB}(y) - \mathcal{E}_\eta^D\{y\} &= A_{CB} - E_{\Omega_{a_1},\eta}^a\{y\} + B_{CB} - E_{\Omega_{a_2},\eta}^a\{y\} + C_{CB} - E_{\Omega_{a_3},\eta}^a\{y\} \\
&\quad + D_{CB} - E_{\Omega_{a_4},\eta}^a\{y\} + G_{CB} - E_{\Omega_*,\eta}\{y\} - E_{\Gamma,\eta}\{y\} \\
&= \varepsilon^2 \sum_{K \subset T_{\Omega_{a_1}}} \phi(\nabla y(m_K)\eta) - \varepsilon^2 \sum_{\ell_1=1}^{N^*-2} \sum_{\ell_2=1}^N \phi(\bar{D}_\eta y(x_{\ell_1}, x_{\ell_2})) \\
&\quad + \varepsilon^2 \sum_{K \subset T_{\Omega_{a_2}}} \phi(\nabla y(m_K)\eta) - \varepsilon^2 \sum_{\ell_1=N^*-1}^{N^{**}-1} \sum_{\ell_2=1}^{N^*-2} \phi(\bar{D}_\eta y(x_{\ell_1}, x_{\ell_2})) \\
&\quad + \varepsilon^2 \sum_{K \subset T_{\Omega_{a_3}}} \phi(\nabla y(m_K)\eta) - \varepsilon^2 \sum_{\ell_1=N^*-1}^{N^{**}-1} \sum_{\ell_2=N^{**}}^N \phi(\bar{D}_\eta y(x_{\ell_1}, x_{\ell_2})) \\
&\quad + \varepsilon^2 \sum_{K \subset T_{\Omega_{a_4}}} \phi(\nabla y(m_K)\eta) - \varepsilon^2 \sum_{\ell_1=N^{**}}^N \sum_{\ell_2=1}^N \phi(\bar{D}_\eta y(x_{\ell_1}, x_{\ell_2})) \\
&\quad + \varepsilon^2 \sum_{K \subset T_{\Omega_*}} \phi(\nabla y(m_K)\eta) - \varepsilon^2 \sum_{K \subset T_{\Omega_*}} \phi(\nabla y(m_K)\eta) + O(\varepsilon^2) \\
&\quad - E_{\Gamma,\eta}\{y\}.
\end{aligned} \tag{4.28}$$

In the sequel we will further work on the error equation by considering separately the errors in each sub-domain  $\Omega_{a_1}$ ,  $\Omega_{a_2}$ ,  $\Omega_{a_3}$  and  $\Omega_{a_4}$ . We will focus first on the terms consisting of the atomistic energy. In each of the terms our aim is to create symmetries involving terms

$$\phi(\bar{D}_\eta y(x_{\ell_1}, x_{\ell_2})) + \phi(\bar{D}_\eta y(x_{\ell_1+1}, x_{\ell_2})) + \phi(\bar{D}_\eta y(x_{\ell_1}, x_{\ell_2+1})) + \phi(\bar{D}_\eta y(x_{\ell_1+1}, x_{\ell_2+1}))$$

so that we can apply Lemmas 20- 22 to obtain (4.71) and in Section 4.6.1 to obtain a satisfactory order for the energy consistency. The remaining terms will involve boundary terms, interface terms and terms connecting the sub-domains  $\Omega_j$ ,  $j =$

$a_1 \cdots, a_4$ . We start by observing,

$$\begin{aligned}
E_{\Omega_{a_1}, \eta}^a \{y\} &= \varepsilon^2 \sum_{\ell_1=1}^{N^*-2} \sum_{\ell_2=1}^N \phi(\overline{D}_\eta y(x_{\ell_1}, x_{\ell_2})) \\
&= \frac{\varepsilon^2}{4} \sum_{\ell_1=1}^{N^*-3} \sum_{\ell_2=1}^{N-1} \{ \phi(\overline{D}_\eta y(x_{\ell_1}, x_{\ell_2})) + \phi(\overline{D}_\eta y(x_{\ell_1+1}, x_{\ell_2})) \\
&\quad + \phi(\overline{D}_\eta y(x_{\ell_1}, x_{\ell_2+1})) + \phi(\overline{D}_\eta y(x_{\ell_1+1}, x_{\ell_2+1})) \} \\
&\quad + \frac{\varepsilon^2}{4} \sum_{\ell_2=1}^{N-1} \{ \phi(\overline{D}_\eta y(x_1, x_{\ell_2})) + \phi(\overline{D}_\eta y(x_1, x_{\ell_2+1})) \} \\
&\quad + \frac{\varepsilon^2}{4} \sum_{\ell_1=1}^{N^*-3} \{ \phi(\overline{D}_\eta y(x_{\ell_1}, x_1)) + \phi(\overline{D}_\eta y(x_{\ell_1+1}, x_1)) \} \\
&\quad + \frac{\varepsilon^2}{4} \sum_{\ell_1=1}^{N^*-3} \{ \phi(\overline{D}_\eta y(x_{\ell_1}, x_N)) + \phi(\overline{D}_\eta y(x_{\ell_1+1}, x_N)) \} \\
&\quad + \frac{\varepsilon^2}{4} \sum_{\ell_2=1}^{N^*-3} \{ \phi(\overline{D}_\eta y(x_{N^*-2}, x_{\ell_2})) + \phi(\overline{D}_\eta y(x_{N^*-2}, x_{\ell_2+1})) \} \\
&\quad + \frac{\varepsilon^2}{4} \sum_{\ell_2=N^*-2}^{N^{**}-1} \{ \phi(\overline{D}_\eta y(x_{N^*-2}, x_{\ell_2})) + \phi(\overline{D}_\eta y(x_{N^*-2}, x_{\ell_2+1})) \} \\
&\quad + \frac{\varepsilon^2}{4} \sum_{\ell_2=N^{**}}^{N-1} \{ \phi(\overline{D}_\eta y(x_{N^*-2}, x_{\ell_2})) + \phi(\overline{D}_\eta y(x_{N^*-2}, x_{\ell_2+1})) \} \\
&\quad + \frac{\varepsilon^2}{4} \{ \phi(\overline{D}_\eta y(x_1, x_1)) + \phi(\overline{D}_\eta y(x_1, x_N)) \\
&\quad + \phi(\overline{D}_\eta y(x_{N^*-2}, x_1)) + \phi(\overline{D}_\eta y(x_{N^*-2}, x_N)) \}.
\end{aligned} \tag{4.29}$$

Similarly,

$$\begin{aligned}
E_{\Omega_{a2},\eta}^a\{y\} &= \varepsilon^2 \sum_{\ell_1=N^*-1}^{N^{**}-1} \sum_{\ell_2=1}^{N^*-2} \phi(\overline{D}_\eta y(x_{\ell_1}, x_{\ell_2})) \\
&= \frac{\varepsilon^2}{4} \sum_{\ell_1=N^*-1}^{N^{**}-2} \sum_{\ell_2=1}^{N^*-3} \{ \phi(\overline{D}_\eta y(x_{\ell_1}, x_{\ell_2})) + \phi(\overline{D}_\eta y(x_{\ell_1+1}, x_{\ell_2})) \\
&\quad + \phi(\overline{D}_\eta y(x_{\ell_1}, x_{\ell_2+1})) + \phi(\overline{D}_\eta y(x_{\ell_1+1}, x_{\ell_2+1})) \} \\
&\quad + \frac{\varepsilon^2}{4} \sum_{\ell_2=1}^{N^*-3} \{ \phi(\overline{D}_\eta y(x_{N^*-1}, x_{\ell_2})) + \phi(\overline{D}_\eta y(x_{N^*-1}, x_{\ell_2+1})) \} \\
&\quad + \frac{\varepsilon^2}{4} \sum_{\ell_1=N^*-1}^{N^{**}-2} \{ \phi(\overline{D}_\eta y(x_{\ell_1}, x_1)) + \phi(\overline{D}_\eta y(x_{\ell_1+1}, x_1)) \} \\
&\quad + \frac{\varepsilon^2}{4} \sum_{\ell_1=N^*-1}^{N^{**}-2} \{ \phi(\overline{D}_\eta y(x_{\ell_1}, x_{N^*-2})) + \phi(\overline{D}_\eta y(x_{\ell_1+1}, x_{N^*-2})) \} \\
&\quad + \frac{\varepsilon^2}{4} \sum_{\ell_2=1}^{N^*-3} \{ \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{\ell_2})) + \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{\ell_2+1})) \} \\
&\quad + \frac{\varepsilon^2}{4} \{ \phi(\overline{D}_\eta y(x_{N^*-1}, x_1)) + \phi(\overline{D}_\eta y(x_{N^*-1}, x_{N^*-2})) \\
&\quad + \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_1)) + \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{N^*-2})) \},
\end{aligned} \tag{4.30}$$

and,

$$\begin{aligned}
E_{\Omega_{a3},\eta}^a\{y\} &= \varepsilon^2 \sum_{\ell_1=N^*-1}^{N^{**}-1} \sum_{\ell_2=N^{**}}^N \phi(\overline{D}_\eta y(x_{\ell_1}, x_{\ell_2})) \\
&= \frac{\varepsilon^2}{4} \sum_{\ell_1=N^*-1}^{N^{**}-2} \sum_{\ell_2=N^{**}}^{N-1} \{ \phi(\overline{D}_\eta y(x_{\ell_1}, x_{\ell_2})) + \phi(\overline{D}_\eta y(x_{\ell_1+1}, x_{\ell_2})) \\
&\quad + \phi(\overline{D}_\eta y(x_{\ell_1}, x_{\ell_2+1})) + \phi(\overline{D}_\eta y(x_{\ell_1+1}, x_{\ell_2+1})) \} \\
&\quad + \frac{\varepsilon^2}{4} \sum_{\ell_2=N^{**}}^{N-1} \{ \phi(\overline{D}_\eta y(x_{N^*-1}, x_{\ell_2})) + \phi(\overline{D}_\eta y(x_{N^*-1}, x_{\ell_2+1})) \} \\
&\quad + \frac{\varepsilon^2}{4} \sum_{\ell_1=N^*-1}^{N^{**}-2} \{ \phi(\overline{D}_\eta y(x_{\ell_1}, x_{N^{**}})) + \phi(\overline{D}_\eta y(x_{\ell_1+1}, x_{N^{**}})) \} \\
&\quad + \frac{\varepsilon^2}{4} \sum_{\ell_1=N^*-1}^{N^{**}-2} \{ \phi(\overline{D}_\eta y(x_{\ell_1}, x_N)) + \phi(\overline{D}_\eta y(x_{\ell_1+1}, x_N)) \} \\
&\quad + \frac{\varepsilon^2}{4} \sum_{\ell_2=N^{**}}^{N-1} \{ \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{\ell_2})) + \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{\ell_2+1})) \} \\
&\quad + \frac{\varepsilon^2}{4} \{ \phi(\overline{D}_\eta y(x_{N^*-1}, x_{N^{**}})) + \phi(\overline{D}_\eta y(x_{N^*-1}, x_N)) \\
&\quad + \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{N^{**}})) + \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_N)) \}.
\end{aligned} \tag{4.31}$$

Finally,

$$\begin{aligned}
E_{\Omega_{a_4}, \eta}^a \{y\} &= \varepsilon^2 \sum_{\ell_1=N^{**}}^N \sum_{\ell_2=1}^N \phi(\bar{D}_\eta y(x_{\ell_1}, x_{\ell_2})) \\
&= \frac{\varepsilon^2}{4} \sum_{\ell_1=N^{**}}^{N-1} \sum_{\ell_2=1}^{N-1} \{ \phi(\bar{D}_\eta y(x_{\ell_1}, x_{\ell_2})) + \phi(\bar{D}_\eta y(x_{\ell_1+1}, x_{\ell_2})) \\
&\quad + \phi(\bar{D}_\eta y(x_{\ell_1}, x_{\ell_2+1})) + \phi(\bar{D}_\eta y(x_{\ell_1+1}, x_{\ell_2+1})) \} \\
&\quad + \frac{\varepsilon^2}{4} \sum_{\ell_2=1}^{N^*-3} \{ \phi(\bar{D}_\eta y(x_{N^{**}}, x_{\ell_2})) + \phi(\bar{D}_\eta y(x_{N^{**}}, x_{\ell_2+1})) \} \\
&\quad + \frac{\varepsilon^2}{4} \sum_{\ell_2=N^*-2}^{N^{**}-1} \{ \phi(\bar{D}_\eta y(x_{N^{**}}, x_{\ell_2})) + \phi(\bar{D}_\eta y(x_{N^{**}}, x_{\ell_2+1})) \} \\
&\quad + \frac{\varepsilon^2}{4} \sum_{\ell_2=N^{**}}^{N-1} \{ \phi(\bar{D}_\eta y(x_{N^{**}}, x_{\ell_2})) + \phi(\bar{D}_\eta y(x_{N^{**}}, x_{\ell_2+1})) \} \tag{4.32} \\
&\quad + \frac{\varepsilon^2}{4} \sum_{\ell_1=N^{**}}^{N-1} \{ \phi(\bar{D}_\eta y(x_{\ell_1}, x_1)) + \phi(\bar{D}_\eta y(x_{\ell_1+1}, x_1)) \} \\
&\quad + \frac{\varepsilon^2}{4} \sum_{\ell_1=N^{**}}^{N-1} \{ \phi(\bar{D}_\eta y(x_{\ell_1}, x_N)) + \phi(\bar{D}_\eta y(x_{\ell_1+1}, x_N)) \} \\
&\quad + \frac{\varepsilon^2}{4} \sum_{\ell_2=1}^{N-1} \{ \phi(\bar{D}_\eta y(x_N, x_{\ell_2})) + \phi(\bar{D}_\eta y(x_N, x_{\ell_2+1})) \} \\
&\quad + \frac{\varepsilon^2}{4} \{ \phi(\bar{D}_\eta y(x_{N^{**}}, x_1)) + \phi(\bar{D}_\eta y(x_{N^{**}}, x_N)) \\
&\quad + \phi(\bar{D}_\eta y(x_N, x_1)) + \phi(\bar{D}_\eta y(x_N, x_N)) \}.
\end{aligned}$$

The combined terms corresponding to the inner boundaries of each atomistic region,  $\Omega_{a_1}, \Omega_{a_2}, \Omega_{a_3}$  and  $\Omega_{a_4}$  are given below:

$$\begin{aligned}
& \frac{\varepsilon^2}{4} \sum_{\ell_2=1}^{N^*-3} \{ \phi(\bar{D}_\eta y(x_{N^*-2}, x_{\ell_2})) + \phi(\bar{D}_\eta y(x_{N^*-2}, x_{\ell_2+1})) \} \\
& + \frac{\varepsilon^2}{4} \sum_{\ell_2=N^{**}}^{N-1} \{ \phi(\bar{D}_\eta y(x_{N^*-2}, x_{\ell_2})) + \phi(\bar{D}_\eta y(x_{N^*-2}, x_{\ell_2+1})) \} \\
& + \frac{\varepsilon^2}{4} \sum_{\ell_2=1}^{N^*-3} \{ \phi(\bar{D}_\eta y(x_{N^*-1}, x_{\ell_2})) + \phi(\bar{D}_\eta y(x_{N^*-1}, x_{\ell_2+1})) \} \\
& + \frac{\varepsilon^2}{4} \sum_{\ell_2=1}^{N^*-3} \{ \phi(\bar{D}_\eta y(x_{N^{**}-1}, x_{\ell_2})) + \phi(\bar{D}_\eta y(x_{N^{**}-1}, x_{\ell_2+1})) \} \\
& + \frac{\varepsilon^2}{4} \sum_{\ell_2=N^{**}}^{N-1} \{ \phi(\bar{D}_\eta y(x_{N^*-1}, x_{\ell_2})) + \phi(\bar{D}_\eta y(x_{N^*-1}, x_{\ell_2+1})) \} \\
& + \frac{\varepsilon^2}{4} \sum_{\ell_2=N^{**}}^{N-1} \{ \phi(\bar{D}_\eta y(x_{N^{**}-1}, x_{\ell_2})) + \phi(\bar{D}_\eta y(x_{N^{**}-1}, x_{\ell_2+1})) \} \\
& + \frac{\varepsilon^2}{4} \sum_{\ell_2=1}^{N^*-3} \{ \phi(\bar{D}_\eta y(x_{N^{**}}, x_{\ell_2})) + \phi(\bar{D}_\eta y(x_{N^{**}}, x_{\ell_2+1})) \} \\
& + \frac{\varepsilon^2}{4} \sum_{\ell_2=N^{**}}^{N-1} \{ \phi(\bar{D}_\eta y(x_{N^{**}}, x_{\ell_2})) + \phi(\bar{D}_\eta y(x_{N^{**}}, x_{\ell_2+1})) \} \\
& = \frac{\varepsilon^2}{4} \sum_{\ell_2=1}^{N^*-3} \{ \phi(\bar{D}_\eta y(x_{N^*-2}, x_{\ell_2})) + \phi(\bar{D}_\eta y(x_{N^*-2}, x_{\ell_2+1})) \} \\
& + \phi(\bar{D}_\eta y(x_{N^*-1}, x_{\ell_2})) + \phi(\bar{D}_\eta y(x_{N^*-1}, x_{\ell_2+1})) \} \\
& + \frac{\varepsilon^2}{4} \sum_{\ell_2=N^{**}}^{N-1} \{ \phi(\bar{D}_\eta y(x_{N^*-2}, x_{\ell_2})) + \phi(\bar{D}_\eta y(x_{N^*-2}, x_{\ell_2+1})) \} \\
& + \phi(\bar{D}_\eta y(x_{N^*-1}, x_{\ell_2})) + \phi(\bar{D}_\eta y(x_{N^*-1}, x_{\ell_2+1})) \} \\
& + \frac{\varepsilon^2}{4} \sum_{\ell_2=1}^{N^*-3} \{ \phi(\bar{D}_\eta y(x_{N^{**}-1}, x_{\ell_2})) + \phi(\bar{D}_\eta y(x_{N^{**}-1}, x_{\ell_2+1})) \} \\
& + \phi(\bar{D}_\eta y(x_{N^{**}}, x_{\ell_2})) + \phi(\bar{D}_\eta y(x_{N^{**}}, x_{\ell_2+1})) \} \\
& + \frac{\varepsilon^2}{4} \sum_{\ell_2=N^{**}}^{N-1} \{ \phi(\bar{D}_\eta y(x_{N^{**}-1}, x_{\ell_2})) + \phi(\bar{D}_\eta y(x_{N^{**}-1}, x_{\ell_2+1})) \} \\
& + \phi(\bar{D}_\eta y(x_{N^{**}}, x_{\ell_2})) + \phi(\bar{D}_\eta y(x_{N^{**}}, x_{\ell_2+1})) \}.
\end{aligned} \tag{4.33}$$

Therefore, combining the above, we conclude that

$$\begin{aligned}
E_{\Omega_a, \eta}^a \{y\} &= E_{\Omega_{a_1}, \eta}^a \{y\} + E_{\Omega_{a_2}, \eta}^a \{y\} + E_{\Omega_{a_3}, \eta}^a \{y\} + E_{\Omega_{a_4}, \eta}^a \{y\} \\
&= A_{inner} + A_{ext, B} + A_{\Gamma},
\end{aligned} \tag{4.34}$$

where the terms corresponding to the internal cells are:

$$\begin{aligned}
A_{inner} &= \frac{\varepsilon^2}{4} \sum_{\ell_1=1}^{N^*-3} \sum_{\ell_2=1}^{N-1} \{ \phi(\bar{D}_\eta y(x_{\ell_1}, x_{\ell_2})) + \phi(\bar{D}_\eta y(x_{\ell_1+1}, x_{\ell_2})) + \phi(\bar{D}_\eta y(x_{\ell_1}, x_{\ell_2+1})) \\
&\quad + \phi(\bar{D}_\eta y(x_{\ell_1+1}, x_{\ell_2+1})) \} + \frac{\varepsilon^2}{4} \sum_{\ell_2=1}^{N^*-3} \{ \phi(\bar{D}_\eta y(x_{N^*-2}, x_{\ell_2})) \\
&\quad + \phi(\bar{D}_\eta y(x_{N^*-2}, x_{\ell_2+1})) + \phi(\bar{D}_\eta y(x_{N^*-1}, x_{\ell_2})) + \phi(\bar{D}_\eta y(x_{N^*-1}, x_{\ell_2+1})) \} \\
&\quad + \frac{\varepsilon^2}{4} \sum_{\ell_2=N^{**}}^{N-1} \{ \phi(\bar{D}_\eta y(x_{N^*-2}, x_{\ell_2})) + \phi(\bar{D}_\eta y(x_{N^*-2}, x_{\ell_2+1})) \\
&\quad + \phi(\bar{D}_\eta y(x_{N^*-1}, x_{\ell_2})) + \phi(\bar{D}_\eta y(x_{N^*-1}, x_{\ell_2+1})) \} \\
&\quad + \frac{\varepsilon^2}{4} \sum_{\ell_1=N^*-1}^{N^{**}-2} \sum_{\ell_2=1}^{N^*-3} \{ \phi(\bar{D}_\eta y(x_{\ell_1}, x_{\ell_2})) + \phi(\bar{D}_\eta y(x_{\ell_1+1}, x_{\ell_2})) \\
&\quad + \phi(\bar{D}_\eta y(x_{\ell_1}, x_{\ell_2+1})) + \phi(\bar{D}_\eta y(x_{\ell_1+1}, x_{\ell_2+1})) \} \\
&\quad + \frac{\varepsilon^2}{4} \sum_{\ell_1=N^*-1}^{N^{**}-2} \sum_{\ell_2=N^{**}}^{N-1} \{ \phi(\bar{D}_\eta y(x_{\ell_1}, x_{\ell_2})) + \phi(\bar{D}_\eta y(x_{\ell_1+1}, x_{\ell_2})) \\
&\quad + \phi(\bar{D}_\eta y(x_{\ell_1}, x_{\ell_2+1})) + \phi(\bar{D}_\eta y(x_{\ell_1+1}, x_{\ell_2+1})) \} \\
&\quad + \frac{\varepsilon^2}{4} \sum_{\ell_2=1}^{N^*-3} \{ \phi(\bar{D}_\eta y(x_{N^{**}-1}, x_{\ell_2})) + \phi(\bar{D}_\eta y(x_{N^{**}-1}, x_{\ell_2+1})) \\
&\quad + \phi(\bar{D}_\eta y(x_{N^{**}}, x_{\ell_2})) + \phi(\bar{D}_\eta y(x_{N^{**}}, x_{\ell_2+1})) \} \\
&\quad + \frac{\varepsilon^2}{4} \sum_{\ell_2=N^{**}}^{N-1} \{ \phi(\bar{D}_\eta y(x_{N^{**}-1}, x_{\ell_2})) + \phi(\bar{D}_\eta y(x_{N^{**}-1}, x_{\ell_2+1})) \\
&\quad + \phi(\bar{D}_\eta y(x_{N^{**}}, x_{\ell_2})) + \phi(\bar{D}_\eta y(x_{N^{**}}, x_{\ell_2+1})) \} \\
&\quad + \frac{\varepsilon^2}{4} \sum_{\ell_1=N^{**}}^{N-1} \sum_{\ell_2=1}^{N-1} \{ \phi(\bar{D}_\eta y(x_{\ell_1}, x_{\ell_2})) + \phi(\bar{D}_\eta y(x_{\ell_1+1}, x_{\ell_2})) + \phi(\bar{D}_\eta y(x_{\ell_1}, x_{\ell_2+1})) \\
&\quad + \phi(\bar{D}_\eta y(x_{\ell_1+1}, x_{\ell_2+1})) \},
\end{aligned} \tag{4.35}$$

where we have included the combined terms corresponding to the inner boundaries, from (4.33) of each atomistic region. The terms corresponding to the external boundary are

$$\begin{aligned}
A_{ext,B} = & \frac{\varepsilon^2}{4} \sum_{\ell_2=1}^{N-1} \{ \phi(\overline{D}_\eta y(x_1, x_{\ell_2})) + \phi(\overline{D}_\eta y(x_1, x_{\ell_2+1})) \} \\
& + \frac{\varepsilon^2}{4} \sum_{\ell_1=1}^{N^*-3} \{ \phi(\overline{D}_\eta y(x_{\ell_1}, x_1)) + \phi(\overline{D}_\eta y(x_{\ell_1+1}, x_1)) \} \\
& + \frac{\varepsilon^2}{4} \sum_{\ell_1=1}^{N^*-3} \{ \phi(\overline{D}_\eta y(x_{\ell_1}, x_N)) + \phi(\overline{D}_\eta y(x_{\ell_1+1}, x_N)) \} \\
& + \frac{\varepsilon^2}{4} \{ \phi(\overline{D}_\eta y(x_{N^*-2}, x_1)) + \phi(\overline{D}_\eta y(x_{N^*-2}, x_N)) \} \\
& + \phi(\overline{D}_\eta y(x_1, x_1)) + \phi(\overline{D}_\eta y(x_1, x_N)) \\
& + \frac{\varepsilon^2}{4} \sum_{\ell_1=N^*-1}^{N^{**}-2} \{ \phi(\overline{D}_\eta y(x_{\ell_1}, x_1)) + \phi(\overline{D}_\eta y(x_{\ell_1+1}, x_1)) \} \\
& + \frac{\varepsilon^2}{4} \phi(\overline{D}_\eta y(x_{N^*-1}, x_1)) + \frac{\varepsilon^2}{4} \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_1)) \\
& + \frac{\varepsilon^2}{4} \sum_{\ell_1=N^*-1}^{N^{**}-2} \{ \phi(\overline{D}_\eta y(x_{\ell_1}, x_N)) + \phi(\overline{D}_\eta y(x_{\ell_1+1}, x_N)) \} \\
& + \frac{\varepsilon^2}{4} \phi(\overline{D}_\eta y(x_{N^*-1}, x_N)) + \frac{\varepsilon^2}{4} \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_N)) \\
& + \frac{\varepsilon^2}{4} \sum_{\ell_1=N^{**}}^{N-1} \{ \phi(\overline{D}_\eta y(x_{\ell_1}, x_1)) + \phi(\overline{D}_\eta y(x_{\ell_1+1}, x_1)) \} \\
& + \frac{\varepsilon^2}{4} \sum_{\ell_1=N^{**}}^{N-1} \{ \phi(\overline{D}_\eta y(x_{\ell_1}, x_N)) + \phi(\overline{D}_\eta y(x_{\ell_1+1}, x_N)) \} \\
& + \frac{\varepsilon^2}{4} \sum_{\ell_2=1}^{N-1} \{ \phi(\overline{D}_\eta y(x_N, x_{\ell_2})) + \phi(\overline{D}_\eta y(x_N, x_{\ell_2+1})) \} \\
& + \frac{\varepsilon^2}{4} \phi(\overline{D}_\eta y(x_{N^{**}}, x_N)) + \frac{\varepsilon^2}{4} \phi(\overline{D}_\eta y(x_{N^{**}}, x_1)) \\
& + \frac{\varepsilon^2}{4} \phi(\overline{D}_\eta y(x_N, x_1)) + \frac{\varepsilon^2}{4} \phi(\overline{D}_\eta y(x_N, x_N)),
\end{aligned} \tag{4.36}$$

The terms around the interface  $A_\Gamma$  are given by (4.41) below. We now focus on  $A_{ext,B}$ .

By appropriately rearranging its terms we have

$$\begin{aligned}
A_{ext,B} = & \frac{\varepsilon^2}{4} \sum_{\ell_2=1}^{N-1} \{ \phi(\overline{D}_\eta y(x_1, x_{\ell_2})) + \phi(\overline{D}_\eta y(x_1, x_{\ell_2+1})) \} \\
& + \frac{\varepsilon^2}{4} \sum_{\ell_2=1}^{N-1} \{ \phi(\overline{D}_\eta y(x_N, x_{\ell_2})) + \phi(\overline{D}_\eta y(x_N, x_{\ell_2+1})) \} \\
& + \frac{\varepsilon^2}{4} \sum_{\ell_1=1}^{N^*-3} \{ \phi(\overline{D}_\eta y(x_{\ell_1}, x_1)) + \phi(\overline{D}_\eta y(x_{\ell_1+1}, x_1)) \} \\
& + \frac{\varepsilon^2}{4} \{ \phi(\overline{D}_\eta y(x_{N^*-2}, x_1)) + \phi(\overline{D}_\eta y(x_{N^*-1}, x_1)) \} \\
& + \frac{\varepsilon^2}{4} \sum_{\ell_1=N^*-1}^{N^{**}-2} \{ \phi(\overline{D}_\eta y(x_{\ell_1}, x_1)) + \phi(\overline{D}_\eta y(x_{\ell_1+1}, x_1)) \} \\
& + \frac{\varepsilon^2}{4} \{ \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_1)) + \phi(\overline{D}_\eta y(x_{N^{**}}, x_1)) \} \\
& + \frac{\varepsilon^2}{4} \sum_{\ell_1=N^{**}}^{N-1} \{ \phi(\overline{D}_\eta y(x_{\ell_1}, x_1)) + \phi(\overline{D}_\eta y(x_{\ell_1+1}, x_1)) \} \\
& + \frac{\varepsilon^2}{4} \sum_{\ell_1=1}^{N^*-3} \{ \phi(\overline{D}_\eta y(x_{\ell_1}, x_N)) + \phi(\overline{D}_\eta y(x_{\ell_1+1}, x_N)) \} \\
& + \frac{\varepsilon^2}{4} \{ \phi(\overline{D}_\eta y(x_{N^*-2}, x_N)) + \phi(\overline{D}_\eta y(x_{N^*-1}, x_N)) \} \\
& + \frac{\varepsilon^2}{4} \sum_{\ell_1=N^*-1}^{N^{**}-2} \{ \phi(\overline{D}_\eta y(x_{\ell_1}, x_N)) + \phi(\overline{D}_\eta y(x_{\ell_1+1}, x_N)) \} \\
& + \frac{\varepsilon^2}{4} \{ \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_N)) + \phi(\overline{D}_\eta y(x_{N^{**}}, x_N)) \} \\
& + \frac{\varepsilon^2}{4} \sum_{\ell_1=N^{**}}^{N-1} \{ \phi(\overline{D}_\eta y(x_{\ell_1}, x_N)) + \phi(\overline{D}_\eta y(x_{\ell_1+1}, x_N)) \} \\
& + \frac{\varepsilon^2}{4} \{ \phi(\overline{D}_\eta y(x_1, x_1)) + \phi(\overline{D}_\eta y(x_1, x_N)) \\
& + \phi(\overline{D}_\eta y(x_N, x_1)) + \phi(\overline{D}_\eta y(x_N, x_N)) \}.
\end{aligned} \tag{4.37}$$



Now, we apply the periodicity condition to the terms that contain  $x_N$ , to yield

$$\begin{aligned}
A_{ext,B} = & \frac{\varepsilon^2}{4} \sum_{\ell_2=1}^{N-1} \{ \phi(\overline{D}_\eta y(x_1, x_{\ell_2})) + \phi(\overline{D}_\eta y(x_1, x_{\ell_2+1})) \} \\
& + \frac{\varepsilon^2}{4} \sum_{\ell_2=1}^{N-1} \{ \phi(\overline{D}_\eta y(x_0, x_{\ell_2})) + \phi(\overline{D}_\eta y(x_0, x_{\ell_2+1})) \} \\
& + \frac{\varepsilon^2}{4} \sum_{\ell_1=1}^{N^*-3} \{ \phi(\overline{D}_\eta y(x_{\ell_1}, x_1)) + \phi(\overline{D}_\eta y(x_{\ell_1+1}, x_1)) \} \\
& + \frac{\varepsilon^2}{4} \{ \phi(\overline{D}_\eta y(x_{N^*-2}, x_1)) + \phi(\overline{D}_\eta y(x_{N^*-1}, x_1)) \} \\
& + \frac{\varepsilon^2}{4} \sum_{\ell_1=N^*-1}^{N^{**}-2} \{ \phi(\overline{D}_\eta y(x_{\ell_1}, x_1)) + \phi(\overline{D}_\eta y(x_{\ell_1+1}, x_1)) \} \\
& + \frac{\varepsilon^2}{4} \{ \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_1)) + \phi(\overline{D}_\eta y(x_{N^{**}}, x_1)) \} \\
& + \frac{\varepsilon^2}{4} \sum_{\ell_1=N^{**}}^{N-1} \{ \phi(\overline{D}_\eta y(x_{\ell_1}, x_1)) + \phi(\overline{D}_\eta y(x_{\ell_1+1}, x_1)) \} \tag{4.38} \\
& + \frac{\varepsilon^2}{4} \sum_{\ell_1=1}^{N^*-3} \{ \phi(\overline{D}_\eta y(x_{\ell_1}, x_0)) + \phi(\overline{D}_\eta y(x_{\ell_1+1}, x_0)) \} \\
& + \frac{\varepsilon^2}{4} \{ \phi(\overline{D}_\eta y(x_{N^*-2}, x_0)) + \phi(\overline{D}_\eta y(x_{N^*-1}, x_0)) \} \\
& + \frac{\varepsilon^2}{4} \sum_{\ell_1=N^*-1}^{N^{**}-2} \{ \phi(\overline{D}_\eta y(x_{\ell_1}, x_0)) + \phi(\overline{D}_\eta y(x_{\ell_1+1}, x_0)) \} \\
& + \frac{\varepsilon^2}{4} \{ \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_0)) + \phi(\overline{D}_\eta y(x_{N^{**}}, x_0)) \} \\
& + \frac{\varepsilon^2}{4} \sum_{\ell_1=N^{**}}^{N-1} \{ \phi(\overline{D}_\eta y(x_{\ell_1}, x_0)) + \phi(\overline{D}_\eta y(x_{\ell_1+1}, x_0)) \} \\
& + \frac{\varepsilon^2}{4} \{ \phi(\overline{D}_\eta y(x_1, x_1)) + \phi(\overline{D}_\eta y(x_1, x_0)) \\
& + \phi(\overline{D}_\eta y(x_0, x_1)) + \phi(\overline{D}_\eta y(x_0, x_0)) \}.
\end{aligned}$$

Hence, we conclude that the external boundary terms simplify to

$$\begin{aligned}
A_{ext,B} = & \frac{\varepsilon^2}{4} \sum_{\ell_2=1}^{N-1} \{ \phi(\overline{D}_\eta y(x_1, x_{\ell_2})) + \phi(\overline{D}_\eta y(x_1, x_{\ell_2+1})) \\
& + \phi(\overline{D}_\eta y(x_0, x_{\ell_2})) + \phi(\overline{D}_\eta y(x_0, x_{\ell_2+1})) \} \\
& + \frac{\varepsilon^2}{4} \sum_{\ell_1=1}^{N-1} \{ \phi(\overline{D}_\eta y(x_{\ell_1}, x_1)) + \phi(\overline{D}_\eta y(x_{\ell_1+1}, x_1)) \\
& + \phi(\overline{D}_\eta y(x_{\ell_1}, x_0)) + \phi(\overline{D}_\eta y(x_{\ell_1+1}, x_0)) \} \\
& + \frac{\varepsilon^2}{4} \{ \phi(\overline{D}_\eta y(x_1, x_1)) + \phi(\overline{D}_\eta y(x_1, x_0)) \\
& + \phi(\overline{D}_\eta y(x_0, x_1)) + \phi(\overline{D}_\eta y(x_0, x_0)) \}.
\end{aligned} \tag{4.39}$$

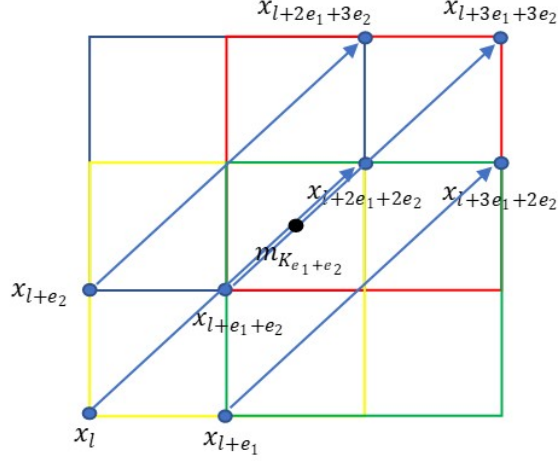
We summarise the analysis so far as follows:

**Lemma 18.** *With the notation introduced in (4.21), (4.27), (4.35), (4.39) and (4.41) we have:*

$$\begin{aligned}
\Phi_\eta^{CB}(y) - \mathcal{E}_\eta^D(y) = & \varepsilon^2 \sum_{K \subset T_{\Omega_{a_1}} \cup T_{\Omega_{a_2}} \cup T_{\Omega_{a_3}} \cup T_{\Omega_{a_4}}} \phi(\nabla y(m_K)\eta) - A_{inner} - A_{ext,B} - A_\Gamma \\
& - E_{\Gamma,\eta}(y) + \mathcal{O}(\varepsilon^2) \\
= & \Theta_B - A_\Gamma - E_{\Gamma,\eta}(y) + \mathcal{O}(\varepsilon^2),
\end{aligned} \tag{4.40}$$

where the remaining terms around the interface  $A_\Gamma$  are given by

$$\begin{aligned}
A_\Gamma = & \frac{\varepsilon^2}{4} \sum_{\ell_1=N^*-1}^{N^{**}-2} \{ \phi(\overline{D}_\eta y(x_{\ell_1}, x_{N^*-2})) + \phi(\overline{D}_\eta y(x_{\ell_1+1}, x_{N^*-2})) \} \\
& + \frac{\varepsilon^2}{4} \sum_{\ell_1=N^*-1}^{N^{**}-2} \{ \phi(\overline{D}_\eta y(x_{\ell_1}, x_{N^{**}})) + \phi(\overline{D}_\eta y(x_{\ell_1+1}, x_{N^{**}})) \} \\
& + \frac{\varepsilon^2}{4} \sum_{\ell_2=N^*-1}^{N^{**}-2} \{ \phi(\overline{D}_\eta y(x_{N^*-2}, x_{\ell_2})) + \phi(\overline{D}_\eta y(x_{N^*-2}, x_{\ell_2+1})) \} \\
& + \frac{\varepsilon^2}{4} \sum_{\ell_2=N^*-1}^{N^{**}-2} \{ \phi(\overline{D}_\eta y(x_{N^{**}}, x_{\ell_2})) + \phi(\overline{D}_\eta y(x_{N^{**}}, x_{\ell_2+1})) \} \\
& + \frac{\varepsilon^2}{4} \{ \phi(\overline{D}_\eta y(x_{N^*-2}, x_{N^{**}})) + \phi(\overline{D}_\eta y(x_{N^*-2}, x_{N^{**}-1})) + \phi(\overline{D}_\eta y(x_{N^*-1}, x_{N^{**}})) \} \\
& + \frac{\varepsilon^2}{4} \{ \phi(\overline{D}_\eta y(x_{N^{**}}, x_{N^{**}-1})) + \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{N^{**}})) + \phi(\overline{D}_\eta y(x_{N^{**}}, x_{N^{**}})) \} \\
& + \frac{\varepsilon^2}{4} \{ \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{N^*-2})) + \phi(\overline{D}_\eta y(x_{N^{**}}, x_{N^*-2})) + \phi(\overline{D}_\eta y(x_{N^{**}}, x_{N^*-1})) \} \\
& + \frac{\varepsilon^2}{4} \{ \phi(\overline{D}_\eta y(x_{N^*-2}, x_{N^*-2})) + \phi(\overline{D}_\eta y(x_{N^*-2}, x_{N^*-1})) \\
& + \phi(\overline{D}_\eta y(x_{N^*-1}, x_{N^*-2})) \}.
\end{aligned} \tag{4.41}$$

Figure 4.2: Displaying  $m_{K_{e_1+e_2}}$ 

#### 4.5.1 Estimate of the bulk terms

To estimate the terms

$$\Theta_B = \varepsilon^2 \sum_{K \subset T_{\Omega_{a_1}} \cup T_{\Omega_{a_2}} \cup T_{\Omega_{a_3}} \cup T_{\Omega_{a_4}}} \phi(\nabla y(m_K)\eta) - A_{inner} - A_{ext,B}, \quad (4.42)$$

we will need some preliminary approximation results which are given in the lemmas below.

**Lemma 19.** *For a smooth function  $y$  and a smooth function  $\phi$  the following holds*

$$\frac{2}{4} \left[ \partial_1 y(m_{1,\ell+e_1}) + \partial_1 y(m_{1,\ell+e_1+2e_2}) + \partial_1 y(m_{1,\ell+e_1+e_2}) + \partial_1 y(m_{1,\ell+e_1+3e_2}) \right] = \quad (4.43)$$

$$2\partial_1 y(m_{K_{e_1+e_2}}) + \mathcal{O}(\varepsilon^2),$$

where  $K_{e_1+e_2}$  represents the cell  $(x_{\ell_1+1}, x_{\ell_1+2}) \times (x_{\ell_2+1}, x_{\ell_2+2})$ ,  $m_{K_{e_1+e_2}}$  is the barycentre of cell  $K_{e_1+e_2}$  and  $m_{1,\ell+e_1}$  is the midpoint of the bottom side of the cell  $K_{e_1} = (x_{\ell_1+1}, x_{\ell_1+2}) \times (x_{\ell_2}, x_{\ell_2+1})$  as displayed in Figures 4.2a and 4.2b along with  $m_{1,\ell+e_1+e_2}$ ,  $m_{1,\ell+e_1+2e_2}$  and  $m_{1,\ell+e_1+3e_2}$ .

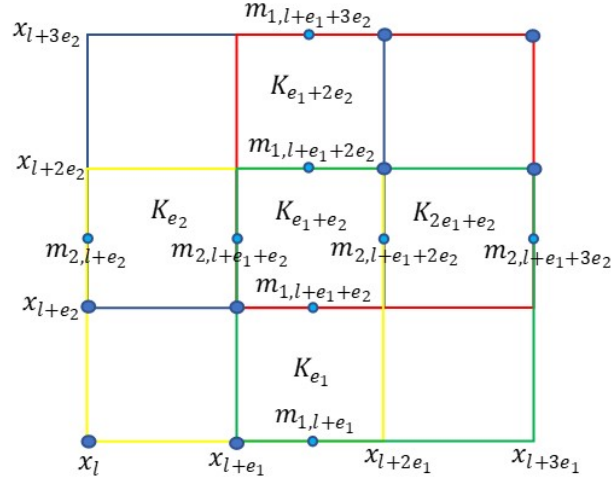
*Proof.* We have,

$$\Phi_\eta^\alpha(y) = \frac{\varepsilon^2}{4} \left[ \sum_{\ell_1=1}^N \sum_{\ell_2=1}^N \left\{ \phi(\overline{D}_\eta y(x_{\ell_1}, x_{\ell_2})) + \phi(\overline{D}_\eta y(x_{\ell_1+1}, x_{\ell_2})) \right. \right. \quad (4.44)$$

$$\left. \left. + \phi(\overline{D}_\eta y(x_{\ell_1}, x_{\ell_2+1})) + \phi(\overline{D}_\eta y(x_{\ell_1+1}, x_{\ell_2+1})) \right\} \right].$$

We create a symmetry around the barycentre  $m_{K_{e_1+e_2}}$  by considering  $\overline{D}_\eta y_\ell$ ,  $\overline{D}_\eta y_{\ell+e_1}$ ,  $\overline{D}_\eta y_{\ell+e_2}$  and  $\overline{D}_\eta y_{\ell+e_1+e_2}$  depicted in Figure 4.3. We introduce the following splittings

$$\overline{D}_\eta y_\ell = \left\{ \frac{1}{2} \overline{D}_{2e_1} y_\ell + \frac{1}{2} \overline{D}_{2e_1} y_{\ell+2e_2} \right\} + \left\{ \frac{1}{2} \overline{D}_{2e_2} y_\ell + \frac{1}{2} \overline{D}_{2e_2} y_{\ell+2e_1} \right\}, \quad (4.45)$$



**Figure 4.3:** Displays  $m_{1,l+e_1}$ ,  $m_{1,l+e_1+e_2}$ ,  $m_{1,l+e_1+2e_2}$  and  $m_{1,l+e_1+3e_2}$ , as well as  $m_{2,l+e_1}$ ,  $m_{2,l+e_1+e_2}$ ,  $m_{2,l+e_1+2e_2}$  and  $m_{2,l+e_1+3e_2}$ .

$$\bar{D}_\eta y_{\ell+e_1} = \left\{ \frac{1}{2} \bar{D}_{2e_1} y_{\ell+e_1} + \frac{1}{2} \bar{D}_{2e_1} y_{\ell+e_1+2e_2} \right\} + \left\{ \frac{1}{2} \bar{D}_{2e_2} y_{\ell+e_1} + \frac{1}{2} \bar{D}_{2e_2} y_{\ell+e_1+2e_1} \right\}, \quad (4.46)$$

$$\bar{D}_\eta y_{\ell+e_2} = \left\{ \frac{1}{2} \bar{D}_{2e_1} y_{\ell+e_2} + \frac{1}{2} \bar{D}_{2e_1} y_{\ell+e_2+2e_2} \right\} + \left\{ \frac{1}{2} \bar{D}_{2e_2} y_{\ell+e_2} + \frac{1}{2} \bar{D}_{2e_2} y_{\ell+e_2+2e_1} \right\}, \quad (4.47)$$

$$\begin{aligned} \bar{D}_\eta y_{\ell+e_1+e_2} = & \left\{ \frac{1}{2} \bar{D}_{2e_1} y_{\ell+e_1+e_2} + \frac{1}{2} \bar{D}_{2e_1} y_{\ell+e_1+3e_2} \right\} + \left\{ \frac{1}{2} \bar{D}_{2e_2} y_{\ell+e_1+e_2} \right. \\ & \left. + \frac{1}{2} \bar{D}_{2e_2} y_{\ell+e_1+3e_2} \right\}. \end{aligned} \quad (4.48)$$

For the following splittings, and due to symmetric differences of the form

$$\frac{u(x+\varepsilon) - u(x-\varepsilon)}{2\varepsilon} = u'(x) + \frac{\varepsilon^2}{6} u^{(3)}(\xi), \quad (4.49)$$

we will get second order approximations for the partial derivatives.

- The first splitting is

$$\frac{1}{2} \bar{D}_{2e_1} y_\ell + \frac{1}{2} \bar{D}_{2e_1} y_{\ell+e_1} = \frac{y_{\ell+2e_1} - y_\ell}{2\varepsilon} + \frac{y_{\ell+3e_1} - y_{\ell+e_1}}{2\varepsilon}. \quad (4.50)$$

By applying the central difference approximation to the terms we have

$$\frac{y_{\ell+3e_1} - y_\ell}{3\varepsilon} = \frac{\partial y(m_{1,l+e_1})}{\partial x_1} + \mathcal{O}(\varepsilon^2), \quad (4.51)$$

and

$$\frac{y_{\ell+2e_1} - y_{\ell+e_1}}{\varepsilon} = \frac{\partial y(m_{1,l+e_1})}{\partial x_1} + \mathcal{O}(\varepsilon^2). \quad (4.52)$$

By substituting these two equations into equation (4.50) we have

$$\begin{aligned} \frac{3}{2} \frac{y_{\ell+3e_1} - y_{\ell}}{3\varepsilon} + \frac{1}{2} \frac{y_{\ell+2e_1} - y_{\ell+e_1}}{\varepsilon} &= \frac{3}{2} \frac{\partial y(m_{1,\ell+e_1})}{\partial x_1} + \frac{1}{2} \frac{\partial y(m_{1,\ell+e_1})}{\partial x_1} + \mathcal{O}(\varepsilon^2) \\ &= 2\partial_1 y(m_{1,\ell+e_1}) + \mathcal{O}(\varepsilon^2). \end{aligned} \quad (4.53)$$

- The second splitting is

$$\frac{1}{2} \overline{D}_{2e_1} y_{\ell+2e_2} + \frac{1}{2} \overline{D}_{2e_1} y_{\ell+e_1+2e_2} = \frac{y_{\ell+2e_1+2e_2} - y_{\ell+2e_2}}{2\varepsilon} + \frac{y_{\ell+3e_1+2e_2} - y_{\ell+e_1+2e_2}}{2\varepsilon}. \quad (4.54)$$

Similarly, we have

$$\frac{y_{\ell+3e_1+2e_2} - y_{\ell+2e_2}}{3\varepsilon} = \frac{\partial y(m_{1,\ell+e_1+2e_2})}{\partial x_1} + \mathcal{O}(\varepsilon^2), \quad (4.55)$$

and

$$\frac{y_{\ell+2e_1+2e_2} - y_{\ell+e_1+2e_2}}{2\varepsilon} = \frac{\partial y(m_{1,\ell+e_1+2e_2})}{\partial x_1} + \mathcal{O}(\varepsilon^2). \quad (4.56)$$

By substituting these two equations into equation (4.54) we have

$$\begin{aligned} \frac{3}{2} \frac{y_{\ell+3e_1+2e_2} - y_{\ell+2e_2}}{3\varepsilon} + \frac{1}{2} \frac{y_{\ell+2e_1+2e_2} - y_{\ell+e_1+2e_2}}{\varepsilon} &= \\ \frac{3}{2} \frac{\partial y(m_{1,\ell+2e_2+e_1})}{\partial x_1} + \frac{1}{2} \frac{\partial y(m_{1,\ell+2e_2+e_1})}{\partial x_1} + \mathcal{O}(\varepsilon^2) &= \\ 2\partial_1 y(m_{1,\ell+2e_2+e_1}) + \mathcal{O}(\varepsilon^2). \end{aligned} \quad (4.57)$$

- The third splitting is

$$\frac{1}{2} \overline{D}_{2e_1} y_{\ell+e_2} + \frac{1}{2} \overline{D}_{2e_1} y_{\ell+e_1+e_2} = \frac{y_{\ell+e_2+2e_1} - y_{\ell+e_2}}{2\varepsilon} + \frac{y_{\ell+3e_1+e_2} - y_{\ell+e_1+e_2}}{2\varepsilon}. \quad (4.58)$$

Thus,

$$\begin{aligned} \frac{3}{2} \frac{y_{\ell+3e_1+e_2} - y_{\ell+e_2}}{3\varepsilon} + \frac{1}{2} \frac{y_{\ell+2e_1+e_2} - y_{\ell+e_1+e_2}}{\varepsilon} &= \\ \frac{3}{2} \frac{\partial y(m_{1,\ell+e_1+e_2})}{\partial x_1} + \frac{1}{2} \frac{\partial y(m_{1,\ell+e_1+e_2})}{\partial x_1} + \mathcal{O}(\varepsilon^2) &= \\ 2\partial_1 y(m_{1,\ell+e_1+e_2}) + \mathcal{O}(\varepsilon^2). \end{aligned} \quad (4.59)$$

- The fourth splitting is

$$\frac{1}{2} \overline{D}_{2e_1} y_{\ell+3e_2} + \frac{1}{2} \overline{D}_{2e_1} y_{\ell+e_1+3e_2} = \frac{y_{\ell+2e_1+3e_2} - y_{\ell+3e_2}}{2\varepsilon} + \frac{y_{\ell+3e_1+3e_2} - y_{\ell+e_1+3e_2}}{2\varepsilon}. \quad (4.60)$$

Similarly,

$$\begin{aligned} \frac{3}{2} \frac{y_{\ell+3e_1+3e_2} - y_{\ell+3e_2}}{3\varepsilon} + \frac{1}{2} \frac{y_{\ell+2e_1+3e_2} - y_{\ell+e_1+3e_2}}{\varepsilon} &= \\ \frac{3}{2} \frac{\partial y(m_{1,\ell+e_1+3e_2})}{\partial x_1} + \frac{1}{2} \frac{\partial y(m_{1,\ell+e_1+3e_2})}{\partial x_1} + \mathcal{O}(\varepsilon^2) &= \\ 2\partial_1 y(m_{1,\ell+e_1+3e_2}) + \mathcal{O}(\varepsilon^2). \end{aligned} \quad (4.61)$$

Hence, by combining equations (4.53), (4.57), (4.59) and (4.61) we obtain

$$\begin{aligned}
& \frac{2}{4} \left[ \partial_1 y(m_{1,\ell+e_1}) + \partial_1 y(m_{1,\ell+e_1+2e_2}) + \partial_1 y(m_{1,\ell+e_1+e_2}) + \partial_1 y(m_{1,\ell+e_1+3e_2}) \right] \\
&= \frac{2}{2} \left( \frac{\partial_1 y(m_{1,\ell+e_1}) + \partial_1 y(m_{1,\ell+e_1+2e_2})}{2} \right) + \frac{2}{2} \left( \frac{\partial_1 y(m_{1,\ell+e_1+e_2}) + \partial_1 y(m_{1,\ell+e_1+3e_2})}{2} \right) \\
&= \partial_1 y(m_{1,\ell+e_1+e_2}) + \partial_1 y(m_{1,\ell+e_1+e_2}) \\
&= 2\partial_1 y(m_{K_{e_1+e_2}}) + \mathcal{O}(\varepsilon^2).
\end{aligned} \tag{4.62}$$

By similar calculations we obtain

$$\begin{aligned}
& \frac{2}{4} \left[ \frac{\partial y(m_{2,\ell+e_2})}{\partial x_2} + \frac{\partial y(m_{2,\ell+2e_1+e_2})}{\partial x_2} + \frac{\partial y(m_{2,\ell+e_1+e_2})}{\partial x_2} + \frac{\partial y(m_{2,\ell+3e_1+e_2})}{\partial x_2} + \mathcal{O}(\varepsilon^2) \right] \\
&= 2 \frac{\partial y(m_{K_{e_1+e_2}})}{\partial x_2} + \mathcal{O}(\varepsilon^2),
\end{aligned} \tag{4.63}$$

where  $m_{2,\ell+e_2}$  is the midpoint of the left side of cell  $K_{e_1}$  as shown in Figures 4.2(a) and (b) along with  $m_{2,\ell+2e_1+e_2}$ ,  $m_{2,\ell+e_1+e_2}$  and  $m_{2,\ell+3e_1+e_2}$ .  $\square$

Lemmas 20-22 are all linked and will be used in Section 4.6.1 and to obtain (4.71).

**Lemma 20.** *For a smooth function  $y$  and a smooth function  $\phi$  whose derivatives are bounded and for a constant  $c \in \mathbb{R}$  we have*

$$\begin{aligned}
& \left| \frac{1}{4} [\phi(\overline{D}_{(2,2)} y_\ell) + \phi(\overline{D}_{(2,2)} y_{\ell+e_1}) + \phi(\overline{D}_{(2,2)} y_{\ell+e_2}) + \phi(\overline{D}_{(2,2)} y_{\ell+e_1+e_2})] \right. \\
& \quad \left. - \phi\left(\frac{\overline{D}_{(2,2)} y_\ell + \overline{D}_{(2,2)} y_{\ell+e_1} + \overline{D}_{(2,2)} y_{\ell+e_2} + \overline{D}_{(2,2)} y_{\ell+e_1+e_2}}{4}\right) \right| \leq c\varepsilon^2.
\end{aligned} \tag{4.64}$$

*Proof.* Since we assumed that  $\phi$  is smooth (Assumption 1) and that its derivatives are bounded (Assumption 3) we can expand  $\phi(a)$ ,  $\phi(b)$ ,  $\phi(c)$  and  $\phi(d)$ , using Taylor

expansion, around  $\left(\frac{a+b+c+d}{4}\right)$  and we obtain

$$\begin{aligned}\phi(a) &= \phi\left(\frac{a+b+c+d}{4}\right) + \phi'\left(\frac{a+b+c+d}{4}\right)\left(\frac{-3a+b+c+d}{4}\right) \\ &\quad + \frac{1}{2}\phi''(\xi_1)\left(\frac{-3a+b+c+d}{4}\right)^2, \\ \phi(b) &= \phi\left(\frac{a+b+c+d}{4}\right) + \phi'\left(\frac{a+b+c+d}{4}\right)\left(\frac{-3b+a+c+d}{4}\right) \\ &\quad + \frac{1}{2}\phi''(\xi_2)\left(\frac{-3b+a+c+d}{4}\right)^2, \\ \phi(c) &= \phi\left(\frac{a+b+c+d}{4}\right) + \phi'\left(\frac{a+b+c+d}{4}\right)\left(\frac{-3c+a+b+d}{4}\right) \\ &\quad + \frac{1}{2}\phi''(\xi_3)\left(\frac{-3c+a+b+d}{4}\right)^2, \\ \phi(d) &= \phi\left(\frac{a+b+c+d}{4}\right) + \phi'\left(\frac{a+b+c+d}{4}\right)\left(\frac{-3d+a+b+c}{4}\right) \\ &\quad + \frac{1}{2}\phi''(\xi_4)\left(\frac{-3d+a+b+c}{4}\right)^2,\end{aligned}$$

where  $\xi_1 \in \left(a, \frac{a+b+c+d}{4}\right)$ ,  $\xi_2$  is between  $b$  and  $\left(\frac{a+b+c+d}{4}\right)$ ,  $\xi_3$  is between  $c$  and  $\left(\frac{a+b+c+d}{4}\right)$  and  $\xi_4 \in \left(\frac{a+b+c+d}{4}, d\right)$ . Adding  $\phi(a)$ ,  $\phi(b)$ ,  $\phi(c)$  and  $\phi(d)$  yields

$$\begin{aligned}\left|\frac{u(a)+u(b)+u(c)+u(d)}{4} - u\left(\frac{a+b+c+d}{4}\right)\right| &\leq c_1[|b-a|^2 + |c-b|^2 + |c-a|^2 \\ &\quad + |d-b|^2 + |d-a|^2 + |d-c|^2].\end{aligned}\tag{4.65}$$

The proof is an application of (4.65) and of the fact the differences of  $\overline{D}_{(2,2)}y_{\ell+e_1}$  and  $\overline{D}_{(2,2)}y_\ell$  are of  $O(\varepsilon)$ , as,

$$|\overline{D}_{(2,2)}y_{\ell+e_1} - \overline{D}_{(2,2)}y_\ell| \leq c\varepsilon, \quad c \in \mathbb{R}.\tag{4.66}$$

Therefore, we conclude,

$$\begin{aligned}&\left|\frac{1}{4}[\phi(\overline{D}_{(2,2)}y_\ell) + \phi(\overline{D}_{(2,2)}y_{\ell+e_1}) + \phi(\overline{D}_{(2,2)}y_{\ell+e_2}) + \phi(\overline{D}_{(2,2)}y_{\ell+e_1+e_2})]\right. \\ &\quad \left.- \phi\left(\frac{\overline{D}_{(2,2)}y_\ell + \overline{D}_{(2,2)}y_{\ell+e_1} + \overline{D}_{(2,2)}y_{\ell+e_2} + \overline{D}_{(2,2)}y_{\ell+e_1+e_2}}{4}\right)\right| \leq c\varepsilon^2, \quad c \in \mathbb{R}.\end{aligned}\tag{4.67}$$

□

It remains to show the following lemma.

**Lemma 21.** *For a smooth function  $y$  and a  $c \in \mathbb{R}$ ,*

$$\left| \frac{\overline{D}_{(2,2)}y_\ell + \overline{D}_{(2,2)}y_{\ell+e_1} + \overline{D}_{(2,2)}y_{\ell+e_2} + \overline{D}_{(2,2)}y_{\ell+e_1+e_2}}{4} - \nabla y(m_{K_{e_1+e_2}}) \binom{2}{2} \right| \leq c\varepsilon^2, \quad (4.68)$$

where  $m_{K_{e_1+e_2}}$  is the barycenter of cell  $K_{e_1+e_2} = (x_{\ell_1+1}, x_{\ell_1+2}) \times (x_{\ell_2+1}, x_{\ell_2+2})$ .

*Proof.* By using the splittings from (4.45)- (4.48) we obtain

$$\begin{aligned} & \left| \frac{1}{4} \left[ \left\{ \frac{1}{2} \overline{D}_{2e_1} y_\ell + \frac{1}{2} \overline{D}_{2e_1} y_{\ell+2e_2} \right\} + \left\{ \frac{1}{2} \overline{D}_{2e_2} y_\ell + \frac{1}{2} \overline{D}_{2e_2} y_{\ell+2e_1} \right\} \right. \right. \\ & + \left\{ \frac{1}{2} \overline{D}_{2e_1} y_{\ell+e_1} + \frac{1}{2} \overline{D}_{2e_1} y_{\ell+e_1+2e_2} \right\} + \left\{ \frac{1}{2} \overline{D}_{2e_2} y_{\ell+e_1} + \frac{1}{2} \overline{D}_{2e_2} y_{\ell+3e_1} \right\} \\ & + \left\{ \frac{1}{2} \overline{D}_{2e_1} y_{\ell+e_2} + \frac{1}{2} \overline{D}_{2e_1} y_{\ell+3e_2} \right\} + \left\{ \frac{1}{2} \overline{D}_{2e_2} y_{\ell+e_2} + \frac{1}{2} \overline{D}_{2e_2} y_{\ell+2e_1+e_2} \right\} \\ & + \left. \left\{ \frac{1}{2} \overline{D}_{2e_1} y_{\ell+e_1+e_2} + \frac{1}{2} \overline{D}_{2e_1} y_{\ell+e_1+3e_2} \right\} + \left\{ \frac{1}{2} \overline{D}_{2e_2} y_{\ell+e_2+e_1} + \frac{1}{2} \overline{D}_{2e_2} y_{\ell+e_2+3e_1} \right\} \right] \right| \leq \\ & \left| \frac{1}{4} \left[ 2 \frac{\partial y(m_{1,\ell+e_1})}{\partial x_1} + 2 \frac{\partial y(m_{1,\ell+e_1+2e_2})}{\partial x_1} + 2 \frac{\partial y(m_{1,\ell+e_1+e_2})}{\partial x_1} + 2 \frac{\partial y(m_{1,\ell+e_1+3e_2})}{\partial x_1} \right. \right. \\ & + \mathcal{O}(\varepsilon^2) \left. \right] + \frac{1}{4} \left[ 2 \frac{\partial y(m_{2,\ell+e_2})}{\partial x_2} + 2 \frac{\partial y(m_{2,\ell+2e_1+e_2})}{\partial x_2} + 2 \frac{\partial y(m_{2,\ell+e_1+e_2})}{\partial x_2} \right. \\ & + \left. 2 \frac{\partial y(m_{2,\ell+3e_1+e_2})}{\partial x_2} + \mathcal{O}(\varepsilon^2) \right] \left| \right| \leq \\ & = \left| 2 \frac{\partial y(m_{K_{e_1+e_2}})}{\partial x_1} + 2 \frac{\partial y(m_{K_{e_1+e_2}})}{\partial x_2} \right| + \mathcal{O}(\varepsilon^2) = \nabla y(m_{K_{e_1+e_2}}) \binom{2}{2} + \mathcal{O}(\varepsilon^2), \end{aligned} \quad (4.69)$$

where the inequality holds due to (4.53), (4.57), (4.59) and (4.61) in Lemma 19 and the equality holds due to 4.62 and 4.63.  $\square$

By applying Taylor expansion to

$$\phi \left( \frac{\overline{D}_{(2,2)}y_\ell + \overline{D}_{(2,2)}y_{\ell+e_1} + \overline{D}_{(2,2)}y_{\ell+e_2} + \overline{D}_{(2,2)}y_{\ell+e_1+e_2}}{4} \right)$$

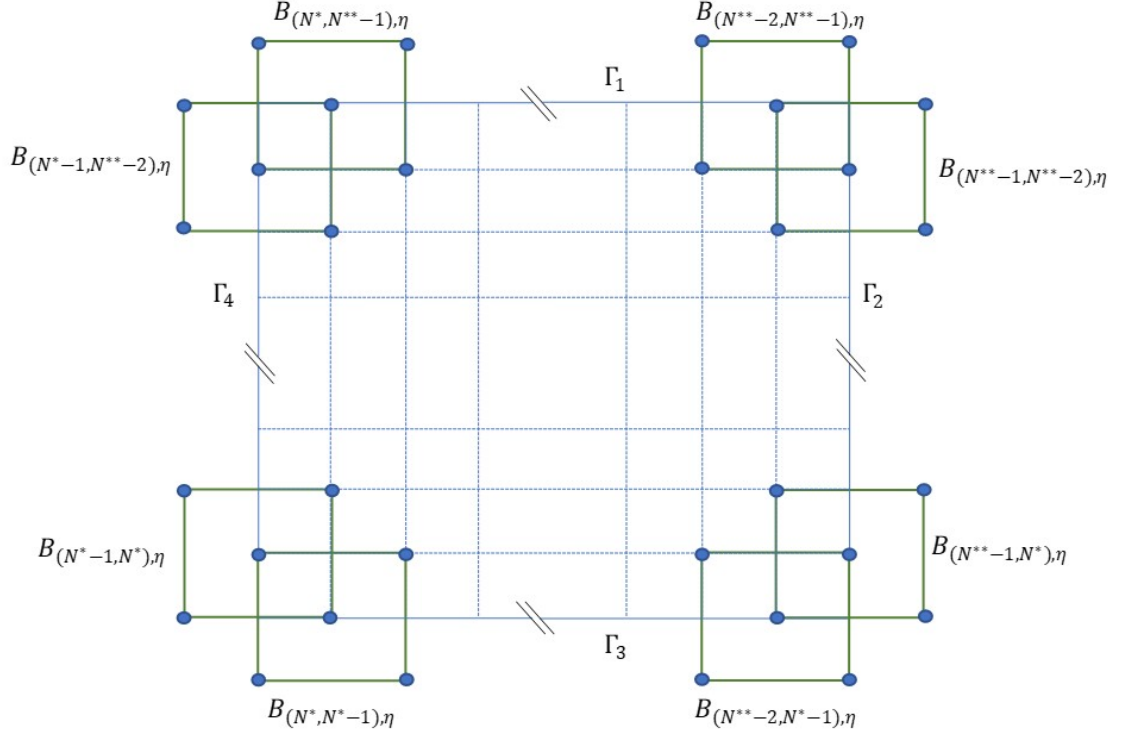
around  $\phi \left( \nabla y(m_{K_{e_1+e_2}}) \binom{2}{2} \right)$  and using similar steps as in Lemma 3 in Chapter 2 as well as Lemma 21 we obtain Lemma 22 below.

**Lemma 22.** *For smooth functions  $y$  and  $\phi$ , a  $c \in \mathbb{R}$  and since Lemma 21 holds we obtain*

$$\left| \phi \left( \frac{\overline{D}_{(2,2)}y_\ell + \overline{D}_{(2,2)}y_{\ell+e_1} + \overline{D}_{(2,2)}y_{\ell+e_2} + \overline{D}_{(2,2)}y_{\ell+e_1+e_2}}{4} \right) - \phi \left( \nabla y(m_{K_{e_1+e_2}}) \binom{2}{2} \right) \right| \leq c\varepsilon^2, \quad (4.70)$$

where  $m_{K_{e_1+e_2}}$  is the barycenter of cell  $K_{e_1+e_2} = (x_{\ell_1+1}, x_{\ell_1+2}) \times (x_{\ell_2+1}, x_{\ell_2+2})$ .





**Figure 4.4:** The bond volumes intersecting the sides of the interface  $\Gamma = \Gamma_1 \cup \Gamma_2 \cup \Gamma_3 \cup \Gamma_4$

By applying Lemmas 20-22 to 4.42 we conclude that

$$\begin{aligned}
 \Theta_B = & \varepsilon^2 \sum_{\ell_2=N^*-1}^{N^{**}} \phi(\nabla y(m_{(N^*-1, \ell_2)})\eta) + \varepsilon^2 \sum_{\ell_1=N^*}^{N^{**}-1} \phi(\nabla y(m_{(\ell_1, N^{**})})\eta) \\
 & + \varepsilon^2 \sum_{\ell_2=N^*-1}^{N^{**}} \phi(\nabla y(m_{(N^{**}, \ell_2)})\eta) + \varepsilon^2 \sum_{\ell_1=N^*}^{N^{**}-1} \phi(\nabla y(m_{(\ell_1, N^*-1)})\eta) + \mathcal{O}(\varepsilon^2).
 \end{aligned} \tag{4.71}$$

## 4.6 Energy on the interfaces

The energy over the bond volumes that intersect with the sides of the interface,  $E_{\Gamma_1}, E_{\Gamma_2}, E_{\Gamma_3}$ , and  $E_{\Gamma_4}$  and the corners of the interface,  $E_{C_1}, E_{C_2}, E_{C_3}$ , and  $E_{C_4}$ , as shown in Figures 4.4, and 4.5, are given below.

The energy of the bond volumes that intersect with interface  $\Gamma_1$ , but not the corners

is

$$\begin{aligned}
E_{\Gamma_1}\{y\} = & \sum_{\ell_1=N^*}^{N^{**}-2} \frac{1}{4} \int_{B_{(\ell_1, N^{**}-1), \eta}} \chi_{\Omega_a} \phi(\bar{D}_\eta y_\ell) dx \\
& - \frac{\varepsilon^2}{4} \sum_{\ell_1=N^*}^{N^{**}-1} \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_{N^{**}-1})) [\bar{D}_{e_2} y(x_{\ell_1}, x_{N^{**}-1}) - \bar{D}_{e_2} y(x_{\ell_1}, x_{N^{**}})] \\
& - \frac{\varepsilon^2}{4} \sum_{\ell_1=N^*}^{N^{**}-1} \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1-2}, x_{N^{**}-1})) [\bar{D}_{e_2} y(x_{\ell_1}, x_{N^{**}-1}) - \bar{D}_{e_2} y(x_{\ell_1}, x_{N^{**}})] \\
& - \frac{\varepsilon^2}{4} \sum_{\ell_1=N^*}^{N^{**}-1} \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_{N^{**}-1})) [\bar{D}_{e_1} y(x_{\ell_1}, x_{N^{**}+1}) - \bar{D}_{e_1} y(x_{\ell_1}, x_{N^{**}-1})] \\
& - \frac{\varepsilon^2}{4} \sum_{\ell_1=N^*}^{N^{**}-1} \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1-1}, x_{N^{**}-1})) [\bar{D}_{e_1} y(x_{\ell_1}, x_{N^{**}+1}) \\
& - \bar{D}_{e_1} y(x_{\ell_1}, x_{N^{**}-1})].
\end{aligned} \tag{4.72}$$

The energy on interface  $\Gamma_2$  but not the corners is

$$\begin{aligned}
E_{\Gamma_2}\{y\} = & \sum_{\ell_2=N^*}^{N^{**}-2} \frac{1}{4} \int_{B_{(N^{**}-1, \ell_2), \eta}} \chi_{\Omega_a} \phi(\bar{D}_\eta y_\ell) dx \\
& - \frac{\varepsilon^2}{4} \sum_{\ell_2=N^*}^{N^{**}-1} \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^{**}-1}, x_{\ell_2})) [\bar{D}_{e_2} y(x_{N^{**}-1}, x_{\ell_2}) - \bar{D}_{e_2} y(x_{N^{**}+1}, x_{\ell_2})] \\
& - \frac{\varepsilon^2}{4} \sum_{\ell_2=N^*}^{N^{**}-1} \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^{**}-1}, x_{\ell_2-1})) [\bar{D}_{e_2} y(x_{N^{**}-1}, x_{\ell_2}) - \bar{D}_{e_2} y(x_{N^{**}+1}, x_{\ell_2})] \\
& - \frac{\varepsilon^2}{4} \sum_{\ell_2=N^*}^{N^{**}-1} \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^{**}-1}, x_{\ell_2})) [\bar{D}_{e_1} y(x_{N^{**}-1}, x_{\ell_2}) - \bar{D}_{e_1} y(x_{N^{**}}, x_{\ell_2})] \\
& - \frac{\varepsilon^2}{4} \sum_{\ell_2=N^*}^{N^{**}-1} \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^{**}-1}, x_{\ell_2-2})) [\bar{D}_{e_1} y(x_{N^{**}-1}, x_{\ell_2}) - \bar{D}_{e_1} y(x_{N^{**}}, x_{\ell_2})].
\end{aligned} \tag{4.73}$$

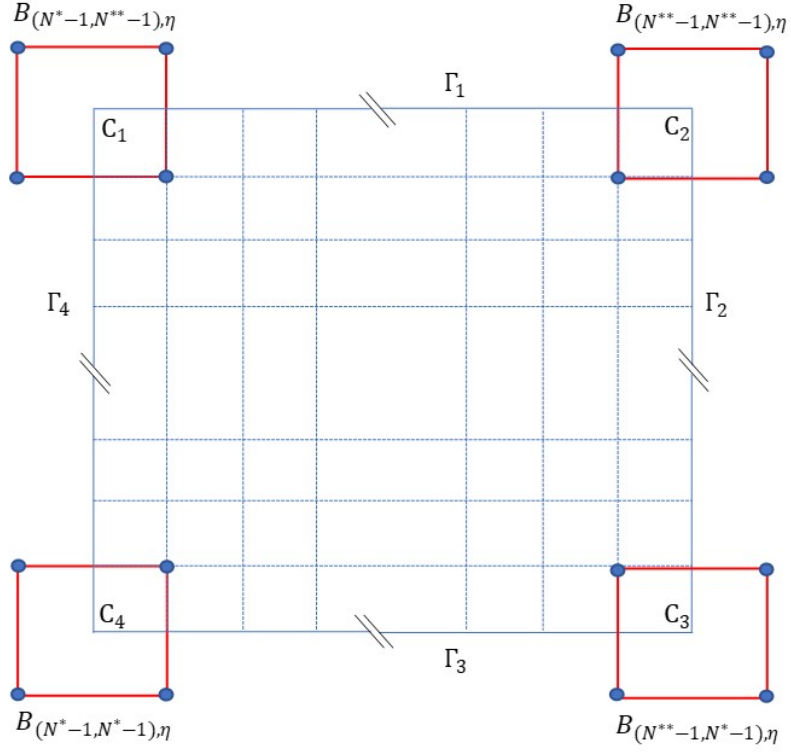
The energy on interface  $\Gamma_3$  but not the corners is

$$\begin{aligned}
E_{\Gamma_3}\{y\} &= \sum_{\ell_1=N^*}^{N^{**}-2} \frac{1}{4} \int_{B_{(\ell_1, N^*-1), \eta}} \chi_{\Omega_a} \phi(\bar{D}_\eta y_\ell) dx \\
&\quad - \frac{\varepsilon^2}{4} \sum_{\ell_1=N^*}^{N^{**}-1} \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_{N^*-1})) [\bar{D}_{e_2} y(x_{\ell_1}, x_{N^*}) - \bar{D}_{e_2} y(x_{\ell_1}, x_{N^*-1})] \\
&\quad - \frac{\varepsilon^2}{4} \sum_{\ell_1=N^*}^{N^{**}-1} \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1-2}, x_{N^*-1})) [\bar{D}_{e_2} y(x_{\ell_1}, x_{N^*}) - \bar{D}_{e_2} y(x_{\ell_1}, x_{N^*-1})] \\
&\quad - \frac{\varepsilon^2}{4} \sum_{\ell_1=N^*}^{N^{**}-1} \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_{N^*-1})) [\bar{D}_{e_1} y(x_{\ell_1}, x_{N^*+1}) - \bar{D}_{e_1} y(x_{\ell_1}, x_{N^*-1})] \\
&\quad - \frac{\varepsilon^2}{4} \sum_{\ell_1=N^*}^{N^{**}-1} \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1-1}, x_{N^*-1})) [\bar{D}_{e_1} y(x_{\ell_1}, x_{N^*+1}) - \bar{D}_{e_1} y(x_{\ell_1}, x_{N^*-1})].
\end{aligned} \tag{4.74}$$

The energy on interface  $\Gamma_4$  but not the corners is

$$\begin{aligned}
E_{\Gamma_4}\{y\} &= \sum_{\ell_2=N^*}^{N^{**}-2} \frac{1}{4} \int_{B_{(N^*-1, \ell_2), \eta}} \chi_{\Omega_a} \phi(\bar{D}_\eta y_\ell) dx \\
&\quad - \frac{\varepsilon^2}{4} \sum_{\ell_2=N^*}^{N^{**}-1} \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^*-1}, x_{\ell_2})) [\bar{D}_{e_2} y(x_{N^*+1}, x_{\ell_2}) - \bar{D}_{e_2} y(x_{N^*-1}, x_{\ell_2})] \\
&\quad - \frac{\varepsilon^2}{4} \sum_{\ell_2=N^*}^{N^{**}-1} \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^*-1}, x_{\ell_2-1})) [\bar{D}_{e_2} y(x_{N^*+1}, x_{\ell_2}) - \bar{D}_{e_2} y(x_{N^*-1}, x_{\ell_2})] \\
&\quad - \frac{\varepsilon^2}{4} \sum_{\ell_2=N^*}^{N^{**}-1} \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^*-1}, x_{\ell_2})) [\bar{D}_{e_1} y(x_{N^*-1}, x_{\ell_2}) - \bar{D}_{e_1} y(x_{N^*}, x_{\ell_2})] \\
&\quad - \frac{\varepsilon^2}{4} \sum_{\ell_2=N^*}^{N^{**}-1} \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^*-1}, x_{\ell_2-2})) [\bar{D}_{e_1} y(x_{N^*-1}, x_{\ell_2}) - \bar{D}_{e_1} y(x_{N^*}, x_{\ell_2})].
\end{aligned} \tag{4.75}$$

The energy of the bond volume on the top left corner where  $\ell = (N^* - 1, N^{**} - 1)$



**Figure 4.5:** The bond volumes intersecting the corners of the interface  $\Gamma = \Gamma_1 \cup \Gamma_2 \cup \Gamma_3 \cup \Gamma_4$

is,

$$\begin{aligned}
 E_{C_1}\{y\} = & \frac{1}{4} \int_{B_{(N^*-1, N^{**}-1), \eta}} \chi_{\Omega_a} \phi(\bar{D}_\eta y_\ell) dx \\
 & + \frac{\varepsilon^2}{4} \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^*-2}, x_{N^{**}-1})) [\bar{D}_{e_2} y(x_{N^*}, x_{N^{**}-1}) - \bar{D}_{e_2} y(x_{N^*}, x_{N^{**}})] \\
 & + \frac{\varepsilon^2}{8} \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^*-1}, x_{N^{**}-1})) [\bar{D}_{e_2} y(x_{N^*-1}, x_{N^{**}}) - \bar{D}_{e_2} y(x_{N^*-1}, x_{N^{**}-1})] \\
 & + \frac{\varepsilon^2}{8} \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^*-1}, x_{N^{**}-1})) [\bar{D}_{e_2} y(x_{N^*+1}, x_{N^{**}-1}) - \bar{D}_{e_2} y(x_{N^*+1}, x_{N^{**}})] \\
 & + \frac{\varepsilon^2}{4} \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^*-1}, x_{N^{**}-2})) [\bar{D}_{e_1} y(x_{N^*-1}, x_{N^{**}}) - \bar{D}_{e_1} y(x_{N^*}, x_{N^{**}})] \\
 & + \frac{\varepsilon^2}{8} \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^*-1}, x_{N^{**}-1})) [\bar{D}_{e_1} y(x_{N^*}, x_{N^{**}-1}) - \bar{D}_{e_1} y(x_{N^*}, x_{N^{**}+1})] \\
 & + \frac{\varepsilon^2}{8} \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^*-1}, x_{N^{**}-1})) [\bar{D}_{e_1} y(x_{N^*-1}, x_{N^{**}+1}) \\
 & - \bar{D}_{e_1} y(x_{N^*-1}, x_{N^{**}-1})].
 \end{aligned} \tag{4.76}$$

The energy of the top right corner where  $\ell = (N^{**} - 1, N^{**} - 1)$  is,

$$\begin{aligned}
E_{C_2}\{y\} = & \frac{1}{4} \int_{B_{(N^{**}-1, N^{**}-1), \eta}} \chi_{\Omega_a} \phi(\overline{D}_\eta y_\ell) dx \\
& + \frac{\varepsilon^2}{4} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-2}, x_{N^{**}-1})) [\overline{D}_{e_2} y(x_{N^{**}}, x_{N^{**}}) - \overline{D}_{e_2} y(x_{N^{**}}, x_{N^{**}-1})] \\
& + \frac{\varepsilon^2}{8} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{N^{**}-1})) [\overline{D}_{e_2} y(x_{N^{**}-1}, x_{N^{**}-1}) \\
& - \overline{D}_{e_2} y(x_{N^{**}-1}, x_{N^{**}})] + \frac{\varepsilon^2}{8} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{N^{**}-1})) \\
& [\overline{D}_{e_2} y(x_{N^{**}+1}, x_{N^{**}-1}) - \overline{D}_{e_2} y(x_{N^{**}+1}, x_{N^{**}})] \\
& + \frac{\varepsilon^2}{4} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{N^{**}-2})) [\overline{D}_{e_1} y(x_{N^{**}}, x_{N^{**}}) - \overline{D}_{e_1} y(x_{N^{**}-1}, x_{N^{**}})] \\
& + \frac{\varepsilon^2}{8} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{N^{**}-1})) [\overline{D}_{e_1} y(x_{N^{**}-1}, x_{N^{**}-1}) \\
& - \overline{D}_{e_1} y(x_{N^{**}-1}, x_{N^{**}+1})] + \frac{\varepsilon^2}{8} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{N^{**}-1})) \\
& [\overline{D}_{e_1} y(x_{N^{**}}, x_{N^{**}+1}) - \overline{D}_{e_1} y(x_{N^{**}}, x_{N^{**}-1})].
\end{aligned} \tag{4.77}$$

The energy of the bottom right corner where  $\ell = (N^{**} - 1, N^* - 1)$  is,

$$\begin{aligned}
E_{C_3}\{y\} = & \frac{1}{4} \int_{B_{(N^{**}-1, N^*-1), \eta}} \chi_{\Omega_a} \phi(\overline{D}_\eta y_\ell) dx \\
& + \frac{\varepsilon^2}{4} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-2}, x_{N^*-1})) [\overline{D}_{e_2} y(x_{N^{**}}, x_{N^*-1}) - \overline{D}_{e_2} y(x_{N^{**}}, x_{N^*})] \\
& + \frac{\varepsilon^2}{8} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{N^*-1})) [\overline{D}_{e_2} y(x_{N^{**}-1}, x_{N^*}) - \overline{D}_{e_2} y(x_{N^{**}-1}, x_{N^*-1})] \\
& + \frac{\varepsilon^2}{8} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{N^*-1})) [\overline{D}_{e_2} y(x_{N^{**}+1}, x_{N^*-1}) - \overline{D}_{e_2} y(x_{N^{**}+1}, x_{N^*})] \\
& + \frac{\varepsilon^2}{4} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{N^*-2})) [\overline{D}_{e_1} y(x_{N^{**}-1}, x_{N^*}) - \overline{D}_{e_1} y(x_{N^{**}}, x_{N^*})] \\
& + \frac{\varepsilon^2}{8} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{N^*-2})) [\overline{D}_{e_1} y(x_{N^{**}-1}, x_{N^*}) - \overline{D}_{e_1} y(x_{N^{**}}, x_{N^*})] \\
& + \frac{\varepsilon^2}{8} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{N^*-1})) [\overline{D}_{e_1} y(x_{N^{**}}, x_{N^*-1}) - \overline{D}_{e_1} y(x_{N^{**}-1}, x_{N^*-1})].
\end{aligned} \tag{4.78}$$

The energy of the bottom left corner where  $\ell = (N^* - 1, N^* - 1)$  is,

$$\begin{aligned}
E_{C_4}\{y\} = & \frac{1}{4} \int_{B_{(N^*-1, N^*-1), \eta}} \chi_{\Omega_a} \phi(\overline{D}_\eta y_\ell) dx \\
& + \frac{\varepsilon^2}{4} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^*-2}, x_{N^*-1})) [\overline{D}_{e_2} y(x_{N^*}, x_{N^*}) - \overline{D}_{e_2} y(x_{N^*}, x_{N^*-1})] \\
& + \frac{\varepsilon^2}{8} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^*-1}, x_{N^*-1})) [\overline{D}_{e_2} y(x_{N^*-1}, x_{N^*-1}) - \overline{D}_{e_2} y(x_{N^*-1}, x_{N^*})] \\
& + \frac{\varepsilon^2}{8} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^*-1}, x_{N^*-1})) [\overline{D}_{e_2} y(x_{N^*+1}, x_{N^*}) - \overline{D}_{e_2} y(x_{N^*+1}, x_{N^*-1})] \\
& + \frac{\varepsilon^2}{4} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^*-1}, x_{N^*-2})) [\overline{D}_{e_1} y(x_{N^*}, x_{N^*}) - \overline{D}_{e_1} y(x_{N^*-1}, x_{N^*})] \\
& + \frac{\varepsilon^2}{8} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^*-1}, x_{N^*-1})) [\overline{D}_{e_1} y(x_{N^*}, x_{N^*+1}) - \overline{D}_{e_1} y(x_{N^*-1}, x_{N^*+1})] \\
& + \frac{\varepsilon^2}{8} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^*-1}, x_{N^*-1})) [\overline{D}_{e_1} y(x_{N^*-1}, x_{N^*-1}) - \overline{D}_{e_1} y(x_{N^*}, x_{N^*-1})].
\end{aligned} \tag{4.79}$$

#### 4.6.1 Final Error equation

We go back to Lemma 18 where we were calculating the difference between the atomistic Cauchy-Born energy and the coupled energy

$$\begin{aligned}
\Phi_\eta^{CB}(y) - \mathcal{E}_\eta^D\{y\} = & \Theta_B - A_\Gamma - E_{\Gamma, \eta}(y) + \mathcal{O}(\varepsilon^2) \\
= & \varepsilon^2 \sum_{\ell_2=N^*-1}^{N^{**}} \phi(\nabla y(m_{(N^*-1, \ell_2)})\eta) + \varepsilon^2 \sum_{\ell_1=N^*}^{N^{**}-1} \phi(\nabla y(m_{(\ell_1, N^{**})})\eta) \\
& + \varepsilon^2 \sum_{\ell_2=N^*-1}^{N^{**}} \phi(\nabla y(m_{(N^{**}, \ell_2)})\eta) + \varepsilon^2 \sum_{\ell_1=N^*}^{N^{**}-1} \phi(\nabla y(m_{(\ell_1, N^*-1)})\eta) \\
& - A_\Gamma - E_{\Gamma, \eta}(y) + \mathcal{O}(\varepsilon^2).
\end{aligned} \tag{4.80}$$

By substituting  $A_\Gamma$  (4.41) into (4.80) and by re-indexing the summations in  $A_\Gamma$  we obtain

$$\begin{aligned}
& \Phi_\eta^{CB}(y) - \mathcal{E}_\eta^D\{y\} = \Theta_B - A_\Gamma - E_{\Gamma,\eta}(y) + \mathcal{O}(\varepsilon^2) \\
& = \varepsilon^2 \sum_{\ell_2=N^*}^{N^{**}-1} \phi(\nabla y(m_{(N^*-1,\ell_2)})\eta) - \frac{\varepsilon^2}{4} \sum_{\ell_2=N^*}^{N^{**}-1} \{\phi(\overline{D}_\eta y(x_{N^*-2}, x_{\ell_2-1})) \\
& \quad + \phi(\overline{D}_\eta y(x_{N^*-2}, x_{\ell_2}))\} + \varepsilon^2 \sum_{\ell_1=N^*}^{N^{**}-1} \phi(\nabla y(m_{(\ell_1, N^{**})})\eta) \\
& \quad - \frac{\varepsilon^2}{4} \sum_{\ell_1=N^*}^{N^{**}-1} \{\phi(\overline{D}_\eta y(x_{\ell_1-1}, x_{N^{**}})) + \phi(\overline{D}_\eta y(x_{\ell_1}, x_{N^{**}}))\} \\
& \quad + \varepsilon^2 \sum_{\ell_2=N^*}^{N^{**}-1} \phi(\nabla y(m_{(N^{**}, \ell_2)})\eta) - \frac{\varepsilon^2}{4} \sum_{\ell_2=N^*}^{N^{**}-1} \{\phi(\overline{D}_\eta y(x_{N^{**}}, x_{\ell_2-1})) \\
& \quad + \phi(\overline{D}_\eta y(x_{N^{**}}, x_{\ell_2}))\} + \varepsilon^2 \sum_{\ell_1=N^*}^{N^{**}-1} \phi(\nabla y(m_{(\ell_1, N^*-1)})\eta) \\
& \quad - \frac{\varepsilon^2}{4} \sum_{\ell_1=N^*}^{N^{**}-1} \{\phi(\overline{D}_\eta y(x_{\ell_1-1}, x_{N^*-2})) + \phi(\overline{D}_\eta y(x_{\ell_1}, x_{N^*-2}))\} \\
& \quad + \varepsilon^2 \phi(\nabla y(m_{(N^*-1, N^{**})})\eta) - \frac{\varepsilon^2}{4} [\phi(\overline{D}_\eta y(x_{N^*-2}, x_{N^{**}})) + \phi(\overline{D}_\eta y(x_{N^*-2}, x_{N^{**}-1})) \\
& \quad + \phi(\overline{D}_\eta y(x_{N^*-1}, x_{N^{**}}))] + \varepsilon^2 \phi(\nabla y(m_{(N^{**}, N^{**})})\eta) - \frac{\varepsilon^2}{4} [\phi(\overline{D}_\eta y(x_{N^{**}}, x_{N^{**}-1})) \\
& \quad + \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{N^{**}})) + \phi(\overline{D}_\eta y(x_{N^{**}}, x_{N^{**}}))] + \varepsilon^2 \phi(\nabla y(m_{(N^{**}, N^*-1)})\eta) \\
& \quad - \frac{\varepsilon^2}{4} [\phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{N^*-2})) + \phi(\overline{D}_\eta y(x_{N^{**}}, x_{N^*-2})) + \phi(\overline{D}_\eta y(x_{N^{**}}, x_{N^*-1}))] \\
& \quad + \varepsilon^2 \phi(\nabla y(m_{(N^*-1, N^*-1)})\eta) - \frac{\varepsilon^2}{4} [\phi(\overline{D}_\eta y(x_{N^*-2}, x_{N^*-2})) + \phi(\overline{D}_\eta y(x_{N^*-2}, x_{N^*-1})) \\
& \quad + \phi(\overline{D}_\eta y(x_{N^*-1}, x_{N^*-2}))] - E_{\Gamma,\eta}(y) + \mathcal{O}(\varepsilon^2).
\end{aligned} \tag{4.81}$$

We have not included  $E_\Gamma$  explicitly because the equation would be very long and so we will refer to equations (4.72)-(4.79). From the interface energy terms in the corners,  $E_{C_1}$ ,  $E_{C_2}$ ,  $E_{C_3}$  and  $E_{C_4}$ , (4.76)-(4.79) we will break down the first term for each corner. For example, for corner  $E_{C_1}$  we will split the first term from

$$\frac{1}{4} \int_{B_{(N^*-1, N^{**}-1), \eta}} \chi_{\Omega_a} \phi(\overline{D}_\eta y_\ell) dx = -\frac{3\varepsilon^2}{4} \phi(\overline{D}_\eta y(x_{N^*-1}, x_{N^{**}-1}))$$

into

$$-\frac{\varepsilon^2}{4} \phi(\overline{D}_\eta y(x_{N^*-1}, x_{N^{**}-1})) \quad \text{and} \quad -\frac{\varepsilon^2}{2} \phi(\overline{D}_\eta y(x_{N^*-1}, x_{N^{**}-1})). \tag{4.82}$$

Then we will join the term  $-\frac{\varepsilon^2}{4}\phi(\overline{D}_\eta y(x_{N^*-1}, x_{N^{**}-1}))$  with the terms

$$\begin{aligned} & \varepsilon^2 \phi(\nabla y(m_{(N^*-1, N^{**})})\eta) - \frac{\varepsilon^2}{4}[\phi(\overline{D}_\eta y(x_{N^*-2}, x_{N^{**}})) + \phi(\overline{D}_\eta y(x_{N^*-2}, x_{N^{**}-1})) \\ & + \phi(\overline{D}_\eta y(x_{N^*-1}, x_{N^{**}}))], \end{aligned} \quad (4.83)$$

from  $\Phi_\eta^{CB}(y) - \mathcal{E}_\eta^D\{y\}$ , (4.81). By applying Lemma 22 we obtain

$$\begin{aligned} & \phi(\nabla y(m_{(N^*-1, N^{**})})\eta) - \frac{1}{4}[\phi(\overline{D}_\eta y(x_{N^*-2}, x_{N^{**}})) + \phi(\overline{D}_\eta y(x_{N^*-2}, x_{N^{**}-1})) \\ & + \phi(\overline{D}_\eta y(x_{N^*-1}, x_{N^{**}})) + \phi(\overline{D}_\eta y(x_{N^*-1}, x_{N^{**}-1}))] = O(\varepsilon^2). \end{aligned} \quad (4.84)$$

Similarly, we repeat these steps for the first terms in  $E_{C_2}$ ,  $E_{C_3}$ ,  $E_{C_4}$  and the respective terms in (4.81). Going back to the  $E_{C_1}$  term that we split into

$$-\frac{\varepsilon^2}{4}\phi(\overline{D}_\eta y(x_{N^*-1}, x_{N^{**}-1})) \quad \text{and} \quad -\frac{\varepsilon^2}{2}\phi(\overline{D}_\eta y(x_{N^*-1}, x_{N^{**}-1})), \quad (4.85)$$

now we will join  $-\frac{\varepsilon^2}{2}\phi(\overline{D}_\eta y(x_{N^*-1}, x_{N^{**}-1}))$  to the first term of the side interface energy  $E_{\Gamma_1}$ ,  $-\frac{\varepsilon^2}{2} \sum_{\ell_1=N^*}^{N^{**}-2} \phi(\overline{D}_\eta y(x_{\ell_1}, x_{N^{**}-1}))$  and we obtain

$$\begin{aligned} & -\frac{\varepsilon^2}{2} \sum_{\ell_1=N^*}^{N^{**}-2} \phi(\overline{D}_\eta y(x_{\ell_1}, x_{N^{**}-1})) - \frac{\varepsilon^2}{2} \phi(\overline{D}_\eta y(x_{N^*-1}, x_{N^{**}-1})) \\ & = -\frac{\varepsilon^2}{2} \sum_{\ell_1=N^*-1}^{N^{**}-2} \phi(\overline{D}_\eta y(x_{\ell_1}, x_{N^{**}-1})). \end{aligned} \quad (4.86)$$

We split the sum in two halves and then we change the index for the second sum into  $\ell'_1 = \ell_1 + 1$  as follows

$$\begin{aligned} & -\frac{\varepsilon^2}{2} \sum_{\ell_1=N^*-1}^{N^{**}-2} \phi(\overline{D}_\eta y(x_{\ell_1}, x_{N^{**}-1})) = -\frac{\varepsilon^2}{4} \sum_{\ell_1=N^*-1}^{N^{**}-2} \phi(\overline{D}_\eta y(x_{\ell_1}, x_{N^{**}-1})) \\ & \quad - \frac{\varepsilon^2}{4} \sum_{\ell_1=N^*-1}^{N^{**}-2} \phi(\overline{D}_\eta y(x_{\ell_1}, x_{N^{**}-1})) \\ & = -\frac{\varepsilon^2}{4} \sum_{\ell_1=N^*-1}^{N^{**}-2} \phi(\overline{D}_\eta y(x_{\ell_1}, x_{N^{**}-1})) \\ & \quad - \frac{\varepsilon^2}{4} \sum_{\ell'_1=N^*}^{N^{**}-1} \phi(\overline{D}_\eta y(x_{\ell'_1-1}, x_{N^{**}-1})). \end{aligned} \quad (4.87)$$



For simplicity we will equate  $\ell'_1 = \ell_1$ . We join these two sums to the corresponding terms on the  $\Gamma_1$  interface energy of  $\Phi_\eta^{CB}(y) - \mathcal{E}_\eta^D\{y\}$  as follows

$$\begin{aligned}
& \varepsilon^2 \sum_{\ell_1=N^*}^{N^{**}-1} \phi(\nabla y(m_{(\ell_1, N^{**})})\eta) - \frac{\varepsilon^2}{4} \sum_{\ell_1=N^*}^{N^{**}-1} \{\phi(\overline{D}_\eta y(x_{\ell_1-1}, x_{N^{**}})) + \phi(\overline{D}_\eta y(x_{\ell_1}, x_{N^{**}}))\} \\
& - \frac{\varepsilon^2}{4} \sum_{\ell_1=N^*-1}^{N^{**}-2} \phi(\overline{D}_\eta y(x_{\ell_1}, x_{N^{**}-1})) - \frac{\varepsilon^2}{4} \sum_{\ell'_1=N^*}^{N^{**}-1} \phi(\overline{D}_\eta y(x_{\ell'_1-1}, x_{N^{**}-1})) \\
& = \varepsilon^2 \sum_{\ell_1=N^*}^{N^{**}-2} \left\{ \phi(\nabla y(m_{(\ell_1, N^{**})})\eta) - \frac{1}{4} \phi(\overline{D}_\eta y(x_{\ell_1-1}, x_{N^{**}})) - \frac{1}{4} \phi(\overline{D}_\eta y(x_{\ell_1}, x_{N^{**}})) \right. \\
& \quad \left. - \frac{1}{4} \phi(\overline{D}_\eta y(x_{\ell_1}, x_{N^{**}-1})) - \frac{1}{4} \phi(\overline{D}_\eta y(x_{\ell_1-1}, x_{N^{**}-1})) \right\} \\
& + \varepsilon^2 \phi(\nabla y(m_{(N^{**}-1, N^{**})})\eta) - \frac{\varepsilon^2}{4} \{\phi(\overline{D}_\eta y(x_{N^{**}-2}, x_{N^{**}})) - \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{N^{**}})) \\
& \quad - \phi(\overline{D}_\eta y(x_{N^*-1}, x_{N^{**}-1})) - \phi(\overline{D}_\eta y(x_{N^{**}-2}, x_{N^{**}-1}))\}.
\end{aligned} \tag{4.88}$$

We repeat these steps similarly for the other side interface energies and we obtain for side interface energy  $E_{\Gamma_2}$

$$\begin{aligned}
& \varepsilon^2 \sum_{\ell_2=N^*}^{N^{**}-1} \phi(\nabla y(m_{(N^{**}, \ell_2)})\eta) - \frac{\varepsilon^2}{4} \sum_{\ell_2=N^*}^{N^{**}-1} \{\phi(\overline{D}_\eta y(x_{N^{**}}, x_{\ell_2-1})) + \phi(\overline{D}_\eta y(x_{N^{**}}, x_{\ell_2}))\} \\
& - \frac{\varepsilon^2}{4} \sum_{\ell_2=N^*}^{N^{**}-1} \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{\ell_2})) - \frac{\varepsilon^2}{4} \sum_{\ell_2=N^*+1}^{N^{**}} \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{\ell_2-1})) \\
& = \varepsilon^2 \sum_{\ell_2=N^*+1}^{N^{**}-1} \left\{ \phi(\nabla y(m_{(N^{**}, \ell_2)})\eta) - \frac{1}{4} \phi(\overline{D}_\eta y(x_{N^{**}}, x_{\ell_2-1})) - \frac{1}{4} \phi(\overline{D}_\eta y(x_{N^{**}}, x_{\ell_2})) \right. \\
& \quad \left. - \frac{1}{4} \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{\ell_2})) - \frac{1}{4} \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{\ell_2-1})) \right\} \\
& + \varepsilon^2 \phi(\nabla y(m_{(N^{**}, N^*-1)})\eta) - \frac{\varepsilon^2}{4} \{\phi(\overline{D}_\eta y(x_{N^{**}}, x_{N^*-1})) - \phi(\overline{D}_\eta y(x_{N^{**}}, x_{N^*})) \\
& \quad - \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{N^*})) - \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{N^{**}-1}))\},
\end{aligned} \tag{4.89}$$

for side interface energy  $E_{\Gamma_3}$

$$\begin{aligned}
& \varepsilon^2 \sum_{\ell_1=N^*}^{N^{**}-1} \phi(\nabla y(m_{(\ell_1, N^*-1)})\eta) - \frac{\varepsilon^2}{4} \sum_{\ell_1=N^*}^{N^{**}-1} \{ \phi(\overline{D}_\eta y(x_{\ell_1-1}, x_{N^*-2})) \\
& + \phi(\overline{D}_\eta y(x_{\ell_1}, x_{N^*-2})) \} - \frac{\varepsilon^2}{4} \sum_{\ell_2=N^*}^{N^{**}-1} \phi(\overline{D}_\eta y(x_{\ell_1}, x_{N^*-1})) \\
& - \frac{\varepsilon^2}{4} \sum_{\ell_1=N^*+1}^{N^{**}} \phi(\overline{D}_\eta y(x_{\ell_1-1}, x_{N^*-1})) \\
& = \varepsilon^2 \sum_{\ell_1=N^*+1}^{N^{**}-1} \{ \phi(\nabla y(m_{(\ell_1, N^*-1)})\eta) - \frac{1}{4} \phi(\overline{D}_\eta y(x_{\ell_1-1}, x_{N^*-2})) - \frac{1}{4} \phi(\overline{D}_\eta y(x_{\ell_1}, x_{N^*-2})) \\
& - \frac{1}{4} \phi(\overline{D}_\eta y(x_{\ell_1}, x_{N^*-1})) - \frac{1}{4} \phi(\overline{D}_\eta y(x_{\ell_1-1}, x_{N^*-1})) \} \\
& + \varepsilon^2 \phi(\nabla y(m_{(N^*, N^*-1)})\eta) - \frac{\varepsilon^2}{4} \{ \phi(\overline{D}_\eta y(x_{N^*-1}, x_{N^*-2})) - \phi(\overline{D}_\eta y(x_{N^*}, x_{N^*-2})) \\
& - \phi(\overline{D}_\eta y(x_{N^*}, x_{N^*-1})) - \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{N^*-1})) \}, \tag{4.90}
\end{aligned}$$

and finally for side interface energy  $E_{\Gamma_4}$

$$\begin{aligned}
& \varepsilon^2 \sum_{\ell_2=N^*}^{N^{**}-1} \phi(\nabla y(m_{(N^*-1, \ell_2)})\eta) - \frac{\varepsilon^2}{4} \sum_{\ell_2=N^*}^{N^{**}-1} \{ \phi(\overline{D}_\eta y(x_{N^*-2}, x_{\ell_2-1})) \\
& + \phi(\overline{D}_\eta y(x_{N^*-2}, x_{\ell_2})) \} - \frac{\varepsilon^2}{4} \sum_{\ell_2=N^*-1}^{N^{**}-2} \phi(\overline{D}_\eta y(x_{N^*-1}, x_{\ell_2})) \\
& - \frac{\varepsilon^2}{4} \sum_{\ell_2=N^*}^{N^{**}-1} \phi(\overline{D}_\eta y(x_{N^*-1}, x_{\ell_2-1})) \\
& = \varepsilon^2 \sum_{\ell_2=N^*}^{N^{**}-2} \{ \phi(\nabla y(m_{(N^*-1, \ell_2)})\eta) - \frac{1}{4} \phi(\overline{D}_\eta y(x_{N^*-2}, x_{\ell_2-1})) - \frac{1}{4} \phi(\overline{D}_\eta y(x_{N^*-2}, x_{\ell_2})) \\
& - \frac{1}{4} \phi(\overline{D}_\eta y(x_{N^*-1}, x_{\ell_2-1})) - \frac{1}{4} \phi(\overline{D}_\eta y(x_{N^*-1}, x_{\ell_2})) \} \\
& + \varepsilon^2 \phi(\nabla y(m_{(N^*-1, N^{**}-1)})\eta) - \frac{\varepsilon^2}{4} \{ \phi(\overline{D}_\eta y(x_{N^*-2}, x_{N^{**}-2})) - \phi(\overline{D}_\eta y(x_{N^*-2}, x_{N^{**}-1})) \\
& - \phi(\overline{D}_\eta y(x_{N^*-1}, x_{N^*-1})) - \phi(\overline{D}_\eta y(x_{N^*-1}, x_{N^{**}-2})) \}. \tag{4.91}
\end{aligned}$$

For the terms in (4.88)-(4.91) that are in the summation we can apply Lemma 22 and conclude that the summation is of order  $O(\varepsilon^2)$ . For the terms without the summation we rearrange some terms from one side interface to the other and then these terms are also of order  $O(\varepsilon^2)$  due to Lemma 22. In summary, we see that all the terms in (4.81) are of order  $O(\varepsilon^2)$  except of the remaining interface and corner energies (4.72)-(4.79) that we have not examined yet. Now, we only need to examine the following remaining side interface and corner interface energy terms:

$$\begin{aligned}
& \frac{\varepsilon^2}{4} \sum_{\ell_1=N^*}^{N^{**}-1} \nabla_{\zeta} \phi(\overline{D}y(x_{\ell_1}, x_{N^{**}-1})) [\overline{D}_{e_2}y(x_{\ell_1}, x_{N^{**}-1}) - \overline{D}_{e_2}y(x_{\ell_1}, x_{N^{**}})] \\
& + \frac{\varepsilon^2}{4} \sum_{\ell_1=N^*}^{N^{**}-1} \nabla_{\zeta} \phi(\overline{D}y(x_{\ell_1-2}, x_{N^{**}-1})) [\overline{D}_{e_2}y(x_{\ell_1}, x_{N^{**}-1}) - \overline{D}_{e_2}y(x_{\ell_1}, x_{N^{**}})] \\
& - \frac{\varepsilon^2}{4} \sum_{\ell_1=N^*}^{N^{**}-1} \nabla_{\zeta} \phi(\overline{D}_{\eta}y(x_{\ell_1}, x_{N^{**}-1})) [\overline{D}_{e_1}y(x_{\ell_1}, x_{N^{**}+1}) - \overline{D}_{e_1}y(x_{\ell_1}, x_{N^{**}-1})] \\
& - \frac{\varepsilon^2}{4} \sum_{\ell_1=N^*}^{N^{**}-1} \nabla_{\zeta} \phi(\overline{D}_{\eta}y(x_{\ell_1-1}, x_{N^{**}-1})) [\overline{D}_{e_1}y(x_{\ell_1}, x_{N^{**}+1}) - \overline{D}_{e_1}y(x_{\ell_1}, x_{N^{**}-1})] \\
& + \frac{\varepsilon^2}{4} \sum_{\ell_2=N^*}^{N^{**}-1} \nabla_{\zeta} \phi(\overline{D}y(x_{N^{**}-1}, x_{\ell_2})) [\overline{D}_{e_2}y(x_{N^{**}-1}, x_{\ell_2}) - \overline{D}_{e_2}y(x_{N^{**}+1}, x_{\ell_2})] \\
& + \frac{\varepsilon^2}{4} \sum_{\ell_2=N^*}^{N^{**}-1} \nabla_{\zeta} \phi(\overline{D}y(x_{N^{**}-1}, x_{\ell_2-1})) [\overline{D}_{e_2}y(x_{N^{**}-1}, x_{\ell_2}) - \overline{D}_{e_2}y(x_{N^{**}+1}, x_{\ell_2})] \\
& - \frac{\varepsilon^2}{4} \sum_{\ell_2=N^*}^{N^{**}-1} \nabla_{\zeta} \phi(\overline{D}_{\eta}y(x_{N^{**}-1}, x_{\ell_2})) [\overline{D}_{e_1}y(x_{N^{**}-1}, x_{\ell_2}) - \overline{D}_{e_1}y(x_{N^{**}}, x_{\ell_2})] \\
& - \frac{\varepsilon^2}{4} \sum_{\ell_2=N^*}^{N^{**}-1} \nabla_{\zeta} \phi(\overline{D}_{\eta}y(x_{N^{**}-1}, x_{\ell_2-2})) [\overline{D}_{e_1}y(x_{N^{**}-1}, x_{\ell_2}) - \overline{D}_{e_1}y(x_{N^{**}}, x_{\ell_2})] \\
& + \frac{\varepsilon^2}{4} \sum_{\ell_1=N^*}^{N^{**}-1} \nabla_{\zeta} \phi(\overline{D}y(x_{\ell_1}, x_{N^*-1})) [\overline{D}_{e_2}y(x_{\ell_1}, x_{N^*}) - \overline{D}_{e_2}y(x_{\ell_1}, x_{N^*-1})] \\
& + \frac{\varepsilon^2}{4} \sum_{\ell_1=N^*}^{N^{**}-1} \nabla_{\zeta} \phi(\overline{D}y(x_{\ell_1-2}, x_{N^*-1})) [\overline{D}_{e_2}y(x_{\ell_1}, x_{N^*}) - \overline{D}_{e_2}y(x_{\ell_1}, x_{N^*-1})] \\
& - \frac{\varepsilon^2}{4} \sum_{\ell_1=N^*}^{N^{**}-1} \nabla_{\zeta} \phi(\overline{D}y(x_{\ell_1}, x_{N^*-1})) [\overline{D}_{e_1}y(x_{\ell_1}, x_{N^*+1}) - \overline{D}_{e_1}y(x_{\ell_1}, x_{N^*-1})] \\
& - \frac{\varepsilon^2}{4} \sum_{\ell_1=N^*}^{N^{**}-1} \nabla_{\zeta} \phi(\overline{D}y(x_{\ell_1-1}, x_{N^*-1})) [\overline{D}_{e_1}y(x_{\ell_1}, x_{N^*+1}) - \overline{D}_{e_1}y(x_{\ell_1}, x_{N^*-1})] \\
& + \frac{\varepsilon^2}{4} \sum_{\ell_2=N^*}^{N^{**}-1} \nabla_{\zeta} \phi(\overline{D}y(x_{N^*-1}, x_{\ell_2})) [\overline{D}_{e_2}y(x_{N^*+1}, x_{\ell_2}) - \overline{D}_{e_2}y(x_{N^*-1}, x_{\ell_2})] \\
& + \frac{\varepsilon^2}{4} \sum_{\ell_2=N^*}^{N^{**}-1} \nabla_{\zeta} \phi(\overline{D}y(x_{N^*-1}, x_{\ell_2-1})) [\overline{D}_{e_2}y(x_{N^*+1}, x_{\ell_2}) - \overline{D}_{e_2}y(x_{N^*-1}, x_{\ell_2})] \\
& - \frac{\varepsilon^2}{4} \sum_{\ell_2=N^*}^{N^{**}-1} \nabla_{\zeta} \phi(\overline{D}_{\eta}y(x_{N^*-1}, x_{\ell_2})) [\overline{D}_{e_1}y(x_{N^*-1}, x_{\ell_2}) - \overline{D}_{e_1}y(x_{N^*}, x_{\ell_2})] \\
& - \frac{\varepsilon^2}{4} \sum_{\ell_2=N^*}^{N^{**}-1} \nabla_{\zeta} \phi(\overline{D}_{\eta}y(x_{N^*-1}, x_{\ell_2-2})) [\overline{D}_{e_1}y(x_{N^*-1}, x_{\ell_2}) - \overline{D}_{e_1}y(x_{N^*}, x_{\ell_2})]
\end{aligned}$$

$$\begin{aligned}
& -\frac{\varepsilon^2}{4}\nabla_\zeta\phi(\overline{D}y(x_{N^*-2}, x_{N^{**}-1}))[\overline{D}_{e_2}y(x_{N^*}, x_{N^{**}-1}) - \overline{D}_{e_2}y(x_{N^*}, x_{N^{**}})] \\
& -\frac{\varepsilon^2}{8}\nabla_\zeta\phi(\overline{D}y(x_{N^*-1}, x_{N^{**}-1}))[\overline{D}_{e_2}y(x_{N^*-1}, x_{N^{**}}) - \overline{D}_{e_2}y(x_{N^*-1}, x_{N^{**}-1})] \\
& -\frac{\varepsilon^2}{8}\nabla_\zeta\phi(\overline{D}y(x_{N^*-1}, x_{N^{**}-1}))[\overline{D}_{e_2}y(x_{N^*+1}, x_{N^{**}-1}) - \overline{D}_{e_2}y(x_{N^*+1}, x_{N^{**}})] \\
& +\frac{\varepsilon^2}{4}\nabla_\zeta\phi(\overline{D}_\eta y(x_{N^*-1}, x_{N^{**}-2}))[\overline{D}_{e_1}y(x_{N^*-1}, x_{N^{**}}) - \overline{D}_{e_1}y(x_{N^*}, x_{N^{**}})] \\
& +\frac{\varepsilon^2}{8}\nabla_\zeta\phi(\overline{D}_\eta y(x_{N^*-1}, x_{N^{**}-1}))[\overline{D}_{e_1}y(x_{N^*}, x_{N^{**}-1}) - \overline{D}_{e_1}y(x_{N^*}, x_{N^{**}+1})] \\
& +\frac{\varepsilon^2}{8}\nabla_\zeta\phi(\overline{D}_\eta y(x_{N^*-1}, x_{N^{**}-1}))[\overline{D}_{e_1}y(x_{N^*-1}, x_{N^{**}+1}) - \overline{D}_{e_1}y(x_{N^*-1}, x_{N^{**}-1})] \\
& -\frac{\varepsilon^2}{4}\nabla_\zeta\phi(\overline{D}y(x_{N^{**}-2}, x_{N^{**}-1}))[\overline{D}_{e_2}y(x_{N^{**}}, x_{N^{**}}) - \overline{D}_{e_2}y(x_{N^{**}}, x_{N^{**}-1})] \\
& -\frac{\varepsilon^2}{8}\nabla_\zeta\phi(\overline{D}y(x_{N^{**}-1}, x_{N^{**}-1}))[\overline{D}_{e_2}y(x_{N^{**}-1}, x_{N^{**}-1}) - \overline{D}_{e_2}y(x_{N^{**}-1}, x_{N^{**}})] \\
& -\frac{\varepsilon^2}{8}\nabla_\zeta\phi(\overline{D}y(x_{N^{**}-1}, x_{N^{**}-1}))[\overline{D}_{e_2}y(x_{N^{**}+1}, x_{N^{**}-1}) - \overline{D}_{e_2}y(x_{N^{**}+1}, x_{N^{**}})] \\
& +\frac{\varepsilon^2}{4}\nabla_\zeta\phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{N^{**}-2}))[\overline{D}_{e_1}y(x_{N^{**}}, x_{N^{**}}) - \overline{D}_{e_1}y(x_{N^{**}-1}, x_{N^{**}})] \\
& +\frac{\varepsilon^2}{8}\nabla_\zeta\phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{N^{**}-1}))[\overline{D}_{e_1}y(x_{N^{**}-1}, x_{N^{**}-1}) - \overline{D}_{e_1}y(x_{N^{**}-1}, x_{N^{**}+1})] \\
& +\frac{\varepsilon^2}{8}\nabla_\zeta\phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{N^{**}-1}))[\overline{D}_{e_1}y(x_{N^{**}}, x_{N^{**}+1}) - \overline{D}_{e_1}y(x_{N^{**}}, x_{N^{**}-1})] \\
& -\frac{\varepsilon^2}{4}\nabla_\zeta\phi(\overline{D}y(x_{N^{**}-2}, x_{N^*-1}))[\overline{D}_{e_2}y(x_{N^{**}}, x_{N^*-1}) - \overline{D}_{e_2}y(x_{N^{**}}, x_{N^*})] \\
& -\frac{\varepsilon^2}{8}\nabla_\zeta\phi(\overline{D}y(x_{N^{**}-1}, x_{N^*-1}))[\overline{D}_{e_2}y(x_{N^{**}-1}, x_{N^*}) - \overline{D}_{e_2}y(x_{N^{**}-1}, x_{N^*-1})] \\
& -\frac{\varepsilon^2}{8}\nabla_\zeta\phi(\overline{D}y(x_{N^{**}-1}, x_{N^*-1}))[\overline{D}_{e_2}y(x_{N^{**}+1}, x_{N^*-1}) - \overline{D}_{e_2}y(x_{N^{**}+1}, x_{N^*})] \\
& +\frac{\varepsilon^2}{4}\nabla_\zeta\phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{N^*-2}))[\overline{D}_{e_1}y(x_{N^{**}-1}, x_{N^*}) - \overline{D}_{e_1}y(x_{N^{**}}, x_{N^*})] \\
& +\frac{\varepsilon^2}{8}\nabla_\zeta\phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{N^*-2}))[\overline{D}_{e_1}y(x_{N^{**}-1}, x_{N^*}) - \overline{D}_{e_1}y(x_{N^{**}}, x_{N^*})] \\
& +\frac{\varepsilon^2}{8}\nabla_\zeta\phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{N^*-1}))[\overline{D}_{e_1}y(x_{N^{**}}, x_{N^*-1}) - \overline{D}_{e_1}y(x_{N^{**}-1}, x_{N^*-1})] \\
& -\frac{\varepsilon^2}{4}\nabla_\zeta\phi(\overline{D}y(x_{N^*-2}, x_{N^*-1}))[\overline{D}_{e_2}y(x_{N^*}, x_{N^*}) - \overline{D}_{e_2}y(x_{N^*}, x_{N^*-1})] \\
& -\frac{\varepsilon^2}{8}\nabla_\zeta\phi(\overline{D}y(x_{N^*-1}, x_{N^*-1}))[\overline{D}_{e_2}y(x_{N^*-1}, x_{N^*-1}) - \overline{D}_{e_2}y(x_{N^*-1}, x_{N^*})] \\
& -\frac{\varepsilon^2}{8}\nabla_\zeta\phi(\overline{D}y(x_{N^*-1}, x_{N^*-1}))[\overline{D}_{e_2}y(x_{N^*+1}, x_{N^*}) - \overline{D}_{e_2}y(x_{N^*+1}, x_{N^*-1})] \\
& +\frac{\varepsilon^2}{4}\nabla_\zeta\phi(\overline{D}_\eta y(x_{N^*-1}, x_{N^*-2}))[\overline{D}_{e_1}y(x_{N^*}, x_{N^*}) - \overline{D}_{e_1}y(x_{N^*-1}, x_{N^*})] \\
& +\frac{\varepsilon^2}{8}\nabla_\zeta\phi(\overline{D}_\eta y(x_{N^*-1}, x_{N^*-1}))[\overline{D}_{e_1}y(x_{N^*}, x_{N^*+1}) - \overline{D}_{e_1}y(x_{N^*-1}, x_{N^*+1})] \\
& +\frac{\varepsilon^2}{8}\nabla_\zeta\phi(\overline{D}_\eta y(x_{N^*-1}, x_{N^*-1}))[\overline{D}_{e_1}y(x_{N^*-1}, x_{N^*-1}) - \overline{D}_{e_1}y(x_{N^*}, x_{N^*-1})].
\end{aligned}$$

(4.92)

To check the order of these remaining terms we will only examine the two following cases

$$\frac{\varepsilon^2}{4} \sum_{\ell_1=N^*}^{N^{**}-1} \nabla_\zeta \phi(\overline{D}_\eta y(x_{\ell_1}, x_{N^{**}-1})) [\overline{D}_{e_2} y(x_{\ell_1}, x_{N^{**}-1}) - \overline{D}_{e_2} y(x_{\ell_1}, x_{N^{**}})], \quad (4.93)$$

and

$$+ \frac{\varepsilon^2}{4} \sum_{\ell_2=N^*}^{N^{**}-1} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{\ell_2})) [\overline{D}_{e_2} y(x_{N^{**}-1}, x_{\ell_2}) - \overline{D}_{e_2} y(x_{N^{**}+1}, x_{\ell_2})]. \quad (4.94)$$

since all the other terms have a similar form. We will examine the terms in the closed brackets by firstly applying a Taylor expansion to  $y(x_{\ell_1}, x_{N^{**}-1})$ ,  $y(x_{N^{**}-1}, x_{\ell_2})$  and  $y(x_{N^{**}+1}, x_{\ell_2})$  as follows

$$\begin{aligned} y(x_{\ell_1}, x_{N^{**}-1}) &= y(x_{\ell_1}, x_{N^{**}}) + \frac{\partial y(x_{\ell_1}, x_{N^{**}})}{\partial x_2} (x_{N^{**}-1} - x_{N^{**}}) \\ &\quad + \frac{1}{2} \frac{\partial^2 y(x_{\ell_1}, \xi_1)}{\partial x_2^2} (x_{N^{**}-1} - x_{N^{**}})^2 \\ &= y(x_{\ell_1}, x_{N^{**}}) - \varepsilon \frac{\partial y(x_{\ell_1}, x_{N^{**}})}{\partial x_2} + \frac{\varepsilon^2}{2} \frac{\partial^2 y(x_{\ell_1}, \xi_1)}{\partial x_2^2}, \end{aligned} \quad (4.95)$$

$$\begin{aligned} y(x_{N^{**}-1}, x_{\ell_2}) &= y(x_{N^{**}}, x_{\ell_2}) + \frac{\partial y(x_{N^{**}}, x_{\ell_2})}{\partial x_1} (x_{N^{**}-1} - x_{N^{**}}) \\ &\quad + \frac{1}{2} \frac{\partial^2 y(\xi_3, x_{\ell_2})}{\partial x_1^2} (x_{N^{**}-1} - x_{N^{**}})^2 \\ &= y(x_{N^{**}}, x_{\ell_2}) - \varepsilon \frac{\partial y(x_{N^{**}}, x_{\ell_2})}{\partial x_1} + \frac{\varepsilon^2}{2} \frac{\partial^2 y(\xi_3, x_{\ell_2})}{\partial x_1^2}, \end{aligned} \quad (4.96)$$

$$\begin{aligned} y(x_{N^{**}+1}, x_{\ell_2}) &= y(x_{N^{**}}, x_{\ell_2}) + \frac{\partial y(x_{N^{**}}, x_{\ell_2})}{\partial x_1} (x_{N^{**}+1} - x_{N^{**}}) \\ &\quad + \frac{1}{2} \frac{\partial^2 y(\xi_4, x_{\ell_2})}{\partial x_1^2} (x_{N^{**}+1} - x_{N^{**}})^2 \\ &= y(x_{N^{**}}, x_{\ell_2}) + \varepsilon \frac{\partial y(x_{N^{**}}, x_{\ell_2})}{\partial x_1} + \frac{\varepsilon^2}{2} \frac{\partial^2 y(\xi_4, x_{\ell_2})}{\partial x_1^2}. \end{aligned} \quad (4.97)$$

After substituting (4.95) to the terms in the closed brackets in (4.93) we obtain

$$\begin{aligned} \overline{D}_{e_2} y(x_{\ell_1}, x_{N^{**}-1}) - \overline{D}_{e_2} y(x_{\ell_1}, x_{N^{**}}) &= \frac{2y(x_{\ell_1}, x_{N^{**}}) - y(x_{\ell_1}, x_{N^{**}-1}) - y(x_{\ell_1}, x_{N^{**}+1})}{\varepsilon} \\ &= \mathcal{O}(\varepsilon). \end{aligned} \quad (4.98)$$

After substituting (4.96)-(4.97) to the terms in the closed brackets in (4.94) we obtain

$$\begin{aligned} \overline{D}_{e_2} y(x_{N^{**}-1}, x_{\ell_2}) - \overline{D}_{e_2} y(x_{N^{**}+1}, x_{\ell_2}) &= \frac{y(x_{N^{**}-1}, x_{\ell_2+1}) - y(x_{N^{**}+1}, x_{\ell_2+1})}{\varepsilon} \\ &\quad + \frac{y(x_{N^{**}+1}, x_{\ell_2}) - y(x_{N^{**}-1}, x_{\ell_2})}{\varepsilon} \\ &= \mathcal{O}(\varepsilon). \end{aligned} \quad (4.99)$$

Similarly, for the  $\overline{D}_{e_1}$  terms,

$$\overline{D}_{e_1}y(x_{\ell_1}, x_{N^{**}+1}) - \overline{D}_{e_1}y(x_{\ell_1}, x_{N^{**}-1}) = \mathcal{O}(\varepsilon), \quad (4.100)$$

and

$$\overline{D}_{e_1}y(x_{N^{**}-1}, x_{\ell_2}) - \overline{D}_{e_1}y(x_{N^{**}}, x_{\ell_2}) = \mathcal{O}(\varepsilon). \quad (4.101)$$

Hence, all the terms in (4.92) are  $O(\varepsilon)$ . We are ready now to prove the following theorem.

**Theorem 5.** (*Energy Consistency*) *Let  $y$  be a smooth function, and  $\mathcal{E}_\eta^D\{y\}$  the coupled energy in (4.19) then there exists a constant  $M_E = M_E(y)$ , such that*

$$|\mathcal{E}_2^D\{y\} - \Phi_2^{CB}(y)| \leq M_E \varepsilon^2. \quad (4.102)$$

*Proof.* Combining the previous estimates we conclude that

$$\mathcal{E}_2^D\{y\} - \Phi_2^{CB}(y) = \varepsilon^2 \sum_{\ell \in \mathcal{L}} \alpha_\ell + \varepsilon^2 \sum_{\ell \in S_\Gamma} \beta_\ell \quad (4.103)$$

where  $\alpha_\ell = \mathcal{O}(\varepsilon^2)$ ,  $\beta_\ell = \mathcal{O}(\varepsilon)$  and  $S_\Gamma$  is the collection of the interface indices. But then  $\sum_{\ell \in S_\Gamma} 1 = \mathcal{O}(1/\varepsilon)$  and hence  $\varepsilon^2 \sum_{\ell \in S_\Gamma} \beta_\ell = \mathcal{O}(\varepsilon^2)$ , and the proof is complete.  $\square$

# Chapter 5

## Two body Variational Energy Theorem in 2D

### 5.1 Chapter Overview

In this chapter we analyse the variational energy for the two dimensional coupled problem. In fact the analysis leads us to the construction of a new discontinuous coupled method. This construction, although similar in spirit to [19] is different both at the design level and in the final form of the coupled method. The key idea is that without specifying the interface, our analysis leads to two types of terms: (a) terms which are  $O(\varepsilon^2)$  and for  $y = y_F$  vanish and (b) terms which are  $O(1)$  even for  $y = y_F = Fx$ . However, the terms in (b) are explicit and they have an appropriate structure which motivates the introduction of the right interface energy terms in order to eliminate their effect. The setting for this chapter is the same as in Chapter 4. In Section 5.2 we compute the difference between the first variation of the coupled energy and the first variation of the atomistic Cauchy-Born energy

$$\langle D\Phi_\eta^{a,CB}(y), v \rangle_\varepsilon - \langle D\mathcal{E}_\eta^D\{y\}, v \rangle_\varepsilon,$$

where

$$\langle D\mathcal{E}_\eta^D\{y\}, v \rangle_\varepsilon = \langle DE_{\Omega_a, \eta}^a\{y\}, v \rangle_\varepsilon + \langle DE_{\Gamma, \eta}^D\{y\}, v \rangle_\varepsilon + \langle DE_{\Omega_*, \eta}^{a,CB}\{y\}, v \rangle_\varepsilon.$$

We first start by calculating

$$\langle D\Phi_\eta^{a,CB}(y), v \rangle_\varepsilon - \langle DE_{\Omega_*, \eta}^a\{y\}, v \rangle_\varepsilon.$$

For convenience we concentrate on the sums containing

$$\frac{1}{2}\{\overline{D}_{e_2}v_\ell + \frac{1}{2}\overline{D}_{e_2}v_{\ell+e_1}\}.$$

Then we convert the terms with  $\overline{D}_{e_2}v_{\ell+e_1}$  into  $\overline{D}_{e_2}v_\ell$  so that all the terms have the same form and we obtain (5.11). After rearranging the sums and applying the periodicity condition we obtain (5.14), which we named  $Z$ . Next we compute the first variations of the atomistic energies from the coupled model and after adding them together we focus only on the terms that include  $\overline{D}_{2e_2}v_\ell$ , which we call  $H$  (5.21). We apply the periodicity conditions and obtain (5.25). Then we substitute

$$\overline{D}_{2e_2}v_\ell = \overline{D}_{e_2}v_\ell + \overline{D}_{e_2}v_{\ell+e_2},$$

and convert all the terms to be of the form  $\overline{D}_{e_2} v_\ell$  so that again all the terms have the same form and this yields (5.28). After applying the periodicity condition,  $H$  simplifies further and we subtract  $H$  from  $Z$ . Then, by applying Lemma 23, some of the terms are  $O(\varepsilon^2)$  and the remaining terms that we obtain are in (5.31), which we name  $W$ . What remains is to subtract from  $W$  the first variation of the energy on the interface. In Section 5.2.1 we compute the first variation of the energy on the interfaces. Recall that in Chapter 1 the energy on the interface is

$$\begin{aligned} E_{\Gamma,\eta}^D\{y\} &= \sum_{\substack{\ell \in \mathcal{L} \\ B_{\ell,\eta} \in B_\Gamma}} \frac{1}{|\eta_1 \eta_2|} \left[ \int_{B_{\ell,\eta}} \chi_{\Omega_a} \phi(\nabla y^{\ell,\eta} \eta) dx - \int_{B_{\ell,\eta} \cap \Gamma} \phi'(\{\nabla y^{\ell,\eta} \eta\}) \cdot [y^{\ell,\eta} \eta] dS \right] \\ &=: E_1 + E_2. \end{aligned}$$

In the two dimensional case the energy on the interface had to be altered. In the  $E_1$  term we replaced  $\phi(\nabla y^{\ell,\eta} \eta)$  with  $\phi(\overline{D}_\eta y_\ell)$  and the  $E_2$  term takes a different form and is explained in Sections 5.2.2 and 5.2.3. The bond volumes that intersect the interface  $\Gamma$  are composed of the bond volumes that intersect the four sides  $\Gamma_1, \Gamma_2, \Gamma_3$  and  $\Gamma_4$  of the interface  $\Gamma$  and the four bond volumes that intersect the four corners of the interface. We take the first variation of  $E_1$  of the energy on each of the four sides of the interface  $\langle DE_{1,\Gamma_1}, v \rangle, \langle DE_{1,\Gamma_2}, v \rangle, \langle DE_{1,\Gamma_3}, v \rangle$  and  $\langle DE_{1,\Gamma_4}, v \rangle$  and the first variation of  $E_1$  of the energy on the four corners  $\langle DE_{1,C_1}, v \rangle, \langle DE_{1,C_2}, v \rangle, \langle DE_{1,C_3}, v \rangle$  and  $\langle DE_{1,C_4}, v \rangle$ . After some substitutions we focus on the  $\overline{D}_{e_2}$  terms and obtain  $\langle DE_{1,\Gamma_1}, v \rangle_{e_2}, \langle DE_{1,\Gamma_2}, v \rangle_{e_2}, \langle DE_{1,\Gamma_3}, v \rangle_{e_2}, \langle DE_{1,\Gamma_4}, v \rangle_{e_2}, \langle DE_{1,C_1}, v \rangle_{e_2}, \langle DE_{1,C_2}, v \rangle_{e_2}, \langle DE_{1,C_3}, v \rangle_{e_2}$  and  $\langle DE_{1,C_4}, v \rangle_{e_2}$  (5.45)-(5.52). In Section 5.2.2 we compute

$$W - \langle DE_{1,\Gamma_1}, v \rangle_{e_2} - \langle DE_{1,\Gamma_2}, v \rangle_{e_2} - \langle DE_{1,\Gamma_3}, v \rangle_{e_2} - \langle DE_{1,\Gamma_4}, v \rangle_{e_2}.$$

We collect the terms along each interface and when collecting the terms on each corner we subtract  $\langle DE_{1,C_1}, v \rangle_{e_2}, \langle DE_{1,C_2}, v \rangle_{e_2}, \langle DE_{1,C_3}, v \rangle_{e_2}$  and  $\langle DE_{1,C_4}, v \rangle_{e_2}$ . So the remaining terms are (5.62)-(5.69). All these terms have to be cancelled out since the aim of the calculations was to achieve a satisfactory error for the first variation between the atomistic Cauchy-Born energy and the coupled energy. To cancel out the terms we need to subtract from the energy on the interface  $E_{\Gamma,\eta}$ , some terms, the  $E_2$  terms, whose first variation cancels with the terms in (5.62)-(5.69).

In Section 5.2.3 we compute the first variation of the energy on the interfaces and the corners without including their first term whose first variation has been computed in Section 5.2.1. Again we focus on the  $\overline{D}_{e_2}$  terms and subtract these variations from (5.62)-(5.69). By applying Taylor expansion we conclude that the terms that remain are  $O(\varepsilon)$ . By following the same analysis for the  $e_1$  direction the terms that remain are again  $O(\varepsilon)$ . Furthermore, we prove Theorem 6 that shows that the variational consistency error for the two dimensional coupled method is bounded by  $(\varepsilon^2 + \varepsilon^{2-\frac{1}{p}})$  in the discrete  $W^{-1,p}$  norm. Notice that the method introduced is ghost-force free. This follows by inserting in the analysis  $y = y_F = Fx$  and observing that the error for the first variation is identically zero in this case. This provides an alternative method of proof to the one presented in [19] for the discontinuous coupled method in Chapter 1.



## 5.2 Variation of Coupled Energy and Continuum Energy

The setting of the coupled energy and the atomistic energy is the same as in Chapter 4, Section 4.4. Again, for this chapter we will fix  $\eta = (2, 2)$ . We will compute the difference between the first variation of the coupled energy and the first variation of the atomistic Cauchy-Born energy as follows

$$\langle D\Phi_\eta^{a,CB}(y), v \rangle_\varepsilon - \langle D\mathcal{E}_\eta^D\{y\}, v \rangle_\varepsilon, \quad (5.1)$$

where

$$\langle D\mathcal{E}_\eta^D\{y\}, v \rangle_\varepsilon = \langle DE_{\Omega_a, \eta}^a\{y\}, v \rangle_\varepsilon + \langle DE_{\Gamma, \eta}^D\{y\}, v \rangle_\varepsilon + \langle DE_{\Omega_*, \eta}^{a,CB}\{y\}, v \rangle_\varepsilon, \quad (5.2)$$

where

$$\begin{aligned} \langle DE_{\Omega_a, \eta}^a\{y\}, v \rangle_\varepsilon &= \langle DE_{\Omega_{a_1}, \eta}^a\{y\}, v \rangle_\varepsilon + \langle DE_{\Omega_{a_2}, \eta}^a\{y\}, v \rangle_\varepsilon \\ &\quad + \langle DE_{\Omega_{a_3}, \eta}^a\{y\}, v \rangle_\varepsilon + \langle DE_{\Omega_{a_4}, \eta}^a\{y\}, v \rangle_\varepsilon, \end{aligned} \quad (5.3)$$

and the interfacial energy will be defined as,

$$\begin{aligned} \langle DE_{\Gamma, \eta}^D\{y\}, v \rangle_\varepsilon &= \langle DE_{\Gamma_1}\{y\}, v \rangle_\varepsilon + \langle DE_{\Gamma_2}\{y\}, v \rangle_\varepsilon + \langle DE_{\Gamma_3}\{y\}, v \rangle_\varepsilon + \langle DE_{\Gamma_4}\{y\}, v \rangle_\varepsilon \\ &\quad + \langle DE_{C_1}\{y\}, v \rangle_\varepsilon + \langle DE_{C_2}\{y\}, v \rangle_\varepsilon + \langle DE_{C_3}\{y\}, v \rangle_\varepsilon \\ &\quad + \langle DE_{C_4}\{y\}, v \rangle_\varepsilon. \end{aligned} \quad (5.4)$$

Recall from Chapter 4 that the atomistic domains are

$$\begin{aligned} T_{\Omega_{a_1}} &= \{[x_1, x_{N^*}] \times [x_1, x_{N+1}]\} \\ T_{\Omega_{a_2}} &= \{[x_{N^*}, x_{N^{**}}] \times [x_1, x_{N^*}]\} \\ T_{\Omega_{a_3}} &= \{[x_{N^*}, x_{N^{**}}] \times [x_{N^{**}}, x_{N+1}]\} \\ T_{\Omega_{a_4}} &= \{[x_{N^{**}}, x_{N+1}] \times [x_1, x_{N+1}]\}, \end{aligned} \quad (5.5)$$

and the atomistic Cauchy-Born domain

$$T_{\Omega_*} = \{[x_{N^*}, x_{N^{**}}] \times [x_{N^*}, x_{N^{**}}]\}. \quad (5.6)$$

We start from the observation, [Section 1.2.4, [21]]

$$\begin{aligned} \langle DE_{\Omega_*, \eta}^a\{y\}, v \rangle_\varepsilon &= \varepsilon^2 \sum_{K \subset T_{\Omega_*}} \{ \nabla_\zeta \phi(\nabla y(m_K) \eta) \eta_1 \} \frac{1}{2} \{ \overline{D}_{e_1} v_\ell + \overline{D}_{e_1} v_{\ell+e_2} \} \\ &\quad + \varepsilon^2 \sum_{K \subset T_{\Omega_*}} \{ \nabla_\zeta \phi(\nabla y(m_K) \eta) \eta_2 \} \frac{1}{2} \{ \overline{D}_{e_2} v_\ell + \overline{D}_{e_2} v_{\ell+e_1} \} + O(\varepsilon^2). \end{aligned} \quad (5.7)$$

We will first compute the difference between the first variation of the fully atomistic Cauchy Born potential energy with the first variation of the atomistic Cauchy Born potential energy at  $\Omega_*$ :

$$\begin{aligned}
\langle D\Phi_\eta^{a,CB}(y) - DE_{\Omega_*,\eta}^a(y), v \rangle_\varepsilon &= 2\varepsilon^2 \sum_{K \subset T} \{ \nabla_\zeta \phi(\nabla y(m_K)\eta) \} \left\{ \frac{1}{2} \overline{D}_{e_1} v_\ell + \frac{1}{2} \overline{D}_{e_1} v_{\ell+e_2} \right\} \\
&\quad + 2\varepsilon^2 \sum_{K \subset T} \{ \nabla_\zeta \phi(\nabla y(m_K)\eta) \} \left\{ \frac{1}{2} \overline{D}_{e_2} v_\ell + \frac{1}{2} \overline{D}_{e_2} v_{\ell+e_1} \right\} \\
&\quad - 2\varepsilon^2 \sum_{K \subset T_{\Omega_*}} \{ \nabla_\zeta \phi(\nabla y(m_K)\eta) \} \left\{ \frac{1}{2} \overline{D}_{e_1} v_\ell + \frac{1}{2} \overline{D}_{e_1} v_{\ell+e_2} \right\} \\
&\quad - 2\varepsilon^2 \sum_{K \subset T_{\Omega_*}} \{ \nabla_\zeta \phi(\nabla y(m_K)\eta) \} \left\{ \frac{1}{2} \overline{D}_{e_2} v_\ell + \frac{1}{2} \overline{D}_{e_2} v_{\ell+e_1} \right\} \\
&=: A + B + C + D.
\end{aligned} \tag{5.8}$$

For the rest of the calculations we will concentrate on the sums containing

$$\left\{ \frac{1}{2} \overline{D}_{e_2} v_\ell + \frac{1}{2} \overline{D}_{e_2} v_{\ell+e_1} \right\}, \tag{5.9}$$

namely  $B$  and  $D$ . The results for the sums containing the  $\overline{D}_{e_1}$  terms will have similar results. Let  $Z = B + D$ , then the remaining terms are

$$\begin{aligned}
Z &= 2\varepsilon^2 \sum_{\ell_1=1}^{N^*-1} \sum_{\ell_2=1}^N \{ \nabla_\zeta \phi(\nabla y(m_{(\ell_1,\ell_2)})\eta) \} \left\{ \frac{1}{2} \overline{D}_{e_2} v_\ell + \frac{1}{2} \overline{D}_{e_2} v_{\ell+e_1} \right\} \\
&\quad + 2\varepsilon^2 \sum_{\ell_1=N^*}^{N^{**}-1} \sum_{\ell_2=1}^{N^*-1} \{ \nabla_\zeta \phi(\nabla y(m_{(\ell_1,\ell_2)})\eta) \} \left\{ \frac{1}{2} \overline{D}_{e_2} v_\ell + \frac{1}{2} \overline{D}_{e_2} v_{\ell+e_1} \right\} \\
&\quad + 2\varepsilon^2 \sum_{\ell_1=N^*}^{N^{**}-1} \sum_{\ell_2=N^{**}}^N \{ \nabla_\zeta \phi(\nabla y(m_{(\ell_1,\ell_2)})\eta) \} \left\{ \frac{1}{2} \overline{D}_{e_2} v_\ell + \frac{1}{2} \overline{D}_{e_2} v_{\ell+e_1} \right\} \\
&\quad + 2\varepsilon^2 \sum_{\ell_1=N^{**}}^N \sum_{\ell_2=1}^N \{ \nabla_\zeta \phi(\nabla y(m_{(\ell_1,\ell_2)})\eta) \} \left\{ \frac{1}{2} \overline{D}_{e_2} v_\ell + \frac{1}{2} \overline{D}_{e_2} v_{\ell+e_1} \right\}.
\end{aligned} \tag{5.10}$$

We will convert the terms with  $\overline{D}_{e_2} v_{\ell+e_1}$  into  $\overline{D}_{e_2} v_\ell$  by changing the index  $\ell$  to  $\ell' = \ell + e_1$ . For simplicity, and convenience we will drop the apostrophe so that  $\ell = \ell'$ . We conclude that

$$\begin{aligned}
Z = & \varepsilon^2 \sum_{\ell_1=1}^{N^*-1} \sum_{\ell_2=1}^N \{ \nabla_{\zeta} \phi(\nabla y(m_{(\ell_1, \ell_2)}) \eta) \} \bar{D}_{e_2} v_{\ell} \\
& + \varepsilon^2 \sum_{\ell_1=2}^{N^*} \sum_{\ell_2=1}^N \{ \nabla_{\zeta} \phi(\nabla y(m_{(\ell_1-1, \ell_2)}) \eta) \} \bar{D}_{e_2} v_{\ell} \\
& + \varepsilon^2 \sum_{\ell_1=N^*}^{N^{**}-1} \sum_{\ell_2=1}^{N^*-1} \{ \nabla_{\zeta} \phi(\nabla y(m_{(\ell_1, \ell_2)}) \eta) \} \bar{D}_{e_2} v_{\ell} \\
& + \varepsilon^2 \sum_{\ell_1=N^*+1}^{N^{**}} \sum_{\ell_2=1}^{N^*-1} \{ \nabla_{\zeta} \phi(\nabla y(m_{(\ell_1-1, \ell_2)}) \eta) \} \bar{D}_{e_2} v_{\ell} \\
& + \varepsilon^2 \sum_{\ell_1=N^*}^{N^{**}-1} \sum_{\ell_2=N^{**}}^N \{ \nabla_{\zeta} \phi(\nabla y(m_{(\ell_1, \ell_2)}) \eta) \} \bar{D}_{e_2} v_{\ell} \\
& + \varepsilon^2 \sum_{\ell_1=N^*+1}^{N^{**}} \sum_{\ell_2=N^{**}}^N \{ \nabla_{\zeta} \phi(\nabla y(m_{(\ell_1-1, \ell_2)}) \eta) \} \bar{D}_{e_2} v_{\ell} \\
& + \varepsilon^2 \sum_{\ell_1=N^{**}}^N \sum_{\ell_2=1}^N \{ \nabla_{\zeta} \phi(\nabla y(m_{(\ell_1, \ell_2)}) \eta) \} \bar{D}_{e_2} v_{\ell} \\
& + \varepsilon^2 \sum_{\ell_1=N^{**}+1}^{N+1} \sum_{\ell_2=1}^N \{ \nabla_{\zeta} \phi(\nabla y(m_{(\ell_1-1, \ell_2)}) \eta) \} \bar{D}_{e_2} v_{\ell}.
\end{aligned} \tag{5.11}$$

Now we rearrange the above equation so that the indexing of the double sums has the form of (5.10), as follows

$$\begin{aligned}
Z = & \varepsilon^2 \sum_{\ell_1=1}^{N^*-1} \sum_{\ell_2=1}^N \{ \{ \nabla_\zeta \phi(\nabla y(m_{(\ell_1, \ell_2)})\eta) \} + \{ \nabla_\zeta \phi(\nabla y(m_{(\ell_1-1, \ell_2)})\eta) \} \} \bar{D}_{e_2} v_\ell \\
& + \varepsilon^2 \sum_{\ell_2=1}^N \{ \{ \nabla_\zeta \phi(\nabla y(m_{(N^*-1, \ell_2)})\eta) \} \bar{D}_{e_2} v(x_{N^*}, x_{\ell_2}) \\
& - \{ \nabla_\zeta \phi(\nabla y(m_{(0, \ell_2)})\eta) \} \bar{D}_{e_2} v(x_1, x_{\ell_2}) \} \\
& + \varepsilon^2 \sum_{\ell_1=N^*}^{N^{**}-1} \sum_{\ell_2=1}^{N^*-1} \{ \{ \nabla_\zeta \phi(\nabla y(m_{(\ell_1, \ell_2)})\eta) \} + \{ \nabla_\zeta \phi(\nabla y(m_{(\ell_1-1, \ell_2)})\eta) \} \} \bar{D}_{e_2} v_\ell \\
& + \varepsilon^2 \sum_{\ell_2=1}^{N^*-1} \{ \{ \nabla_\zeta \phi(\nabla y(m_{(N^{**}-1, \ell_2)})\eta) \} \bar{D}_{e_2} v(x_{N^{**}}, x_{\ell_2}) \\
& - \{ \nabla_\zeta \phi(\nabla y(m_{(N^*-1, \ell_2)})\eta) \} \bar{D}_{e_2} v(x_{N^*}, x_{\ell_2}) \} \\
& + \varepsilon^2 \sum_{\ell_1=N^*}^{N^{**}-1} \sum_{\ell_2=N^{**}}^N \{ \{ \nabla_\zeta \phi(\nabla y(m_{(\ell_1, \ell_2)})\eta) \} + \{ \nabla_\zeta \phi(\nabla y(m_{(\ell_1-1, \ell_2)})\eta) \} \} \bar{D}_{e_2} v_\ell \\
& + \varepsilon^2 \sum_{\ell_2=N^{**}}^N \{ \{ \nabla_\zeta \phi(\nabla y(m_{(N^{**}-1, \ell_2)})\eta) \} \bar{D}_{e_2} v(x_{N^{**}}, x_{\ell_2}) \\
& - \{ \nabla_\zeta \phi(\nabla y(m_{(N^*-1, \ell_2)})\eta) \} \bar{D}_{e_2} v(x_{N^*}, x_{\ell_2}) \} \\
& + \varepsilon^2 \sum_{\ell_1=N^{**}}^N \sum_{\ell_2=1}^N \{ \{ \nabla_\zeta \phi(\nabla y(m_{(\ell_1, \ell_2)})\eta) \} + \{ \nabla_\zeta \phi(\nabla y(m_{(\ell_1-1, \ell_2)})\eta) \} \} \bar{D}_{e_2} v_\ell \\
& + \varepsilon^2 \sum_{\ell_2=1}^N \{ \{ \nabla_\zeta \phi(\nabla y(m_{(N, \ell_2)})\eta) \} \bar{D}_{e_2} v(x_{N+1}, x_{\ell_2}) \\
& - \{ \nabla_\zeta \phi(\nabla y(m_{(N^{**}-1, \ell_2)})\eta) \} \bar{D}_{e_2} v(x_{N^{**}}, x_{\ell_2}) \}.
\end{aligned} \tag{5.12}$$

After some simplifications and due to periodicity, i.e.

$$\nabla_\zeta \phi(\nabla y(m_{(N, \ell_2)})\eta) \bar{D}_{e_2} v(x_{N+1}, x_{\ell_2}) = \{ \nabla_\zeta \phi(\nabla y(m_{(0, \ell_2)})\eta) \} \bar{D}_{e_2} v(x_1, x_{\ell_2}), \tag{5.13}$$

we obtain

$$\begin{aligned}
Z = & \varepsilon^2 \sum_{\ell_1=1}^{N^*-1} \sum_{\ell_2=1}^N \{ \{ \nabla_\zeta \phi(\nabla y(m_{(\ell_1, \ell_2)}) \eta) \} + \{ \nabla_\zeta \phi(\nabla y(m_{(\ell_1-1, \ell_2)}) \eta) \} \} \bar{D}_{e_2} v_\ell \\
& + \varepsilon^2 \sum_{\ell_1=N^*}^{N^{**}-1} \sum_{\ell_2=1}^{N^*-1} \{ \{ \nabla_\zeta \phi(\nabla y(m_{(\ell_1, \ell_2)}) \eta) \} + \{ \nabla_\zeta \phi(\nabla y(m_{(\ell_1-1, \ell_2)}) \eta) \} \} \bar{D}_{e_2} v_\ell \\
& + \varepsilon^2 \sum_{\ell_1=N^*}^{N^{**}-1} \sum_{\ell_2=N^{**}}^N \{ \{ \nabla_\zeta \phi(\nabla y(m_{(\ell_1, \ell_2)}) \eta) \} + \{ \nabla_\zeta \phi(\nabla y(m_{(\ell_1-1, \ell_2)}) \eta) \} \} \bar{D}_{e_2} v_\ell \\
& + \varepsilon^2 \sum_{\ell_1=N^{**}}^N \sum_{\ell_2=1}^N \{ \{ \nabla_\zeta \phi(\nabla y(m_{(\ell_1, \ell_2)}) \eta) \} + \{ \nabla_\zeta \phi(\nabla y(m_{(\ell_1-1, \ell_2)}) \eta) \} \} \bar{D}_{e_2} v_\ell \\
& + \varepsilon^2 \sum_{\ell_2=N^*}^{N^{**}-1} \{ \nabla_\zeta \phi(\nabla y(m_{(N^*-1, \ell_2)}) \eta) \} \bar{D}_{e_2} v(x_{N^*}, x_{\ell_2}) \\
& - \varepsilon^2 \sum_{\ell_2=N^*}^{N^{**}-1} \{ \{ \nabla_\zeta \phi(\nabla y(m_{(N^{**}-1, \ell_2)}) \eta) \} \bar{D}_{e_2} v(x_{N^{**}}, x_{\ell_2}) \}.
\end{aligned} \tag{5.14}$$

We turn now our attention to the terms of the coupled energy at the atomistic region. The first variation of  $E_{\Omega_{a_1}}$ ,  $E_{\Omega_{a_2}}$ ,  $E_{\Omega_{a_3}}$  will be computed next. We first substitute the splitting

$$\bar{D}_\eta v_\ell = \left\{ \frac{1}{2} \bar{D}_{2e_1} v_\ell + \frac{1}{2} \bar{D}_{2e_1} v_{\ell+2e_2} \right\} + \left\{ \frac{1}{2} \bar{D}_{2e_2} v_\ell + \frac{1}{2} \bar{D}_{2e_2} v_{\ell+2e_1} \right\}, \tag{5.15}$$

and then we convert  $\bar{D}_{2e_1} v_{\ell+2e_2}$  and  $\bar{D}_{2e_2} v_{\ell+2e_1}$  into  $\bar{D}_{2e_1} v_\ell$  and  $\bar{D}_{2e_2} v_\ell$  respectively by re-indexing. To convert  $\bar{D}_{2e_1} v_{\ell+2e_2}$  into  $\bar{D}_{2e_1} v_\ell$  we let  $\ell'_2 = \ell_2 + 2$  and to convert  $\bar{D}_{2e_2} v_{\ell+2e_1}$  into  $\bar{D}_{2e_2} v_\ell$  we let  $\ell'_1 = \ell_1 + 2$ . Again, we drop the apostrophes for convenience.

$$\begin{aligned}
\langle DE_{\Omega_{a_1}, \eta}^a \{y\}, v \rangle_\varepsilon &= \varepsilon^2 \sum_{\ell_1=1}^{N^*-2} \sum_{\ell_2=1}^N \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_{\ell_2})) \bar{D}_\eta v_\ell \\
&= \varepsilon^2 \sum_{\ell_1=1}^{N^*-2} \sum_{\ell_2=1}^N \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_{\ell_2})) \left\{ \frac{1}{2} \bar{D}_{2e_1} v_\ell + \frac{1}{2} \bar{D}_{2e_1} v_{\ell+2e_2} \right\} \\
&\quad + \varepsilon^2 \sum_{\ell_1=1}^{N^*-2} \sum_{\ell_2=1}^N \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_{\ell_2})) \left\{ \frac{1}{2} \bar{D}_{2e_2} v_\ell + \frac{1}{2} \bar{D}_{2e_2} v_{\ell+2e_1} \right\} \\
&= \frac{\varepsilon^2}{2} \sum_{\ell_1=1}^{N^*-2} \sum_{\ell_2=1}^N \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_{\ell_2})) \bar{D}_{2e_1} v_\ell \\
&\quad + \frac{\varepsilon^2}{2} \sum_{\ell_1=1}^{N^*-2} \sum_{\ell_2=3}^{N+2} \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_{\ell_2-2})) \bar{D}_{2e_1} v_\ell \\
&\quad + \frac{\varepsilon^2}{2} \sum_{\ell_1=1}^{N^*-2} \sum_{\ell_2=1}^N \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_{\ell_2})) \bar{D}_{2e_2} v_\ell \\
&\quad + \frac{\varepsilon^2}{2} \sum_{\ell_1=3}^{N^*} \sum_{\ell_2=1}^N \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1-2}, x_{\ell_2})) \bar{D}_{2e_2} v_\ell \\
&= \frac{\varepsilon^2}{2} \sum_{\ell_1=1}^{N^*-2} \sum_{\ell_2=1}^N \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_{\ell_2})) + \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_{\ell_2-2})) \} \bar{D}_{2e_1} v_\ell \\
&\quad + \frac{\varepsilon^2}{2} \sum_{\ell_1=1}^{N^*-2} \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_{N-1})) \bar{D}_{2e_1} v(x_{\ell_1}, x_{N+1}) \\
&\quad + \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_N)) \bar{D}_{2e_1} v(x_{\ell_1}, x_{N+2}) \\
&\quad - \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_{-1})) \bar{D}_{2e_1} v(x_{\ell_1}, x_1) \\
&\quad - \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_0)) \bar{D}_{2e_1} v(x_{\ell_1}, x_2) \} \\
&\quad + \frac{\varepsilon^2}{2} \sum_{\ell_1=1}^{N^*-2} \sum_{\ell_2=1}^N \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_{\ell_2})) \\
&\quad + \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1-2}, x_{\ell_2})) \} \bar{D}_{2e_2} v_\ell \\
&\quad + \frac{\varepsilon^2}{2} \sum_{\ell_2=1}^N \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^*-2}, x_{\ell_2})) \bar{D}_{2e_2} v(x_{N^*}, x_{\ell_2}) \\
&\quad + \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^*-3}, x_{\ell_2})) \bar{D}_{2e_2} v(x_{N^*-1}, x_{\ell_2}) \\
&\quad - \nabla_\zeta \phi(\bar{D}_\eta y(x_{-1}, x_{\ell_2})) \bar{D}_{2e_2} v(x_1, x_{\ell_2}) \\
&\quad - \nabla_\zeta \phi(\bar{D}_\eta y(x_0, x_{\ell_2})) \bar{D}_{2e_2} v(x_2, x_{\ell_2}) \}.
\end{aligned} \tag{5.16}$$

By following similar calculations as in (5.16) yields,

$$\begin{aligned}
\langle DE_{\Omega_{a_2}, \eta}^a \{y\}, v \rangle_\varepsilon &= \varepsilon^2 \sum_{\ell_1=N^*-1}^{N^{**}-1} \sum_{\ell_2=1}^{N^*-2} \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_{\ell_2})) \bar{D}_\eta v_\ell \\
&= \frac{\varepsilon^2}{2} \sum_{\ell_1=N^*-1}^{N^{**}-1} \sum_{\ell_2=1}^{N^*-2} \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_{\ell_2})) \\
&\quad + \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_{\ell_2-2})) \} \bar{D}_{2e_1} v_\ell \\
&\quad + \frac{\varepsilon^2}{2} \sum_{\ell_1=N^*-1}^{N^{**}-1} \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_{N^*-2})) \bar{D}_{2e_1} v(x_{\ell_1}, x_{N^*}) \\
&\quad + \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_{N^*-3})) \bar{D}_{2e_1} v(x_{\ell_1}, x_{N^*-1}) \\
&\quad - \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_{-1})) \bar{D}_{2e_1} v(x_{\ell_1}, x_1) \\
&\quad - \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_0)) \bar{D}_{2e_1} v(x_{\ell_1}, x_2) \} \\
&\quad + \frac{\varepsilon^2}{2} \sum_{\ell_1=N^*-1}^{N^{**}-1} \sum_{\ell_2=1}^{N^*-2} \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_{\ell_2})) \\
&\quad + \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1-2}, x_{\ell_2})) \} \bar{D}_{2e_2} v_\ell \\
&\quad + \frac{\varepsilon^2}{2} \sum_{\ell_2=1}^{N^*-2} \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^{**}-1}, x_{\ell_2})) \bar{D}_{2e_2} v(x_{N^{**}+1}, x_{\ell_2}) \\
&\quad + \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^{**}-2}, x_{\ell_2})) \bar{D}_{2e_2} v(x_{N^{**}}, x_{\ell_2}) \\
&\quad - \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^*-2}, x_{\ell_2})) \bar{D}_{2e_2} v(x_{N^*}, x_{\ell_2}) \\
&\quad - \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^*-3}, x_{\ell_2})) \bar{D}_{2e_2} v(x_{N^*-1}, x_{\ell_2}) \}.
\end{aligned} \tag{5.17}$$

Similarly,

$$\begin{aligned}
\langle DE_{\Omega_{a_3}, \eta}^a \{y\}, v \rangle_\varepsilon &= \varepsilon^2 \sum_{\ell_1=N^*-1}^{N^{**}-1} \sum_{\ell_2=N^{**}}^N \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_{\ell_2})) \bar{D}_\eta v_\ell \\
&= \frac{\varepsilon^2}{2} \sum_{\ell_1=N^*-1}^{N^{**}-1} \sum_{\ell_2=N^{**}}^N \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_{\ell_2})) \\
&\quad + \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_{\ell_2-2})) \} \bar{D}_{2e_1} v_\ell \\
&\quad + \frac{\varepsilon^2}{2} \sum_{\ell_1=N^*-1}^{N^{**}-1} \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_N)) \bar{D}_{2e_1} v(x_{\ell_1}, x_{N+2}) \\
&\quad + \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_{N-1})) \bar{D}_{2e_1} v(x_{\ell_1}, x_{N+1}) \\
&\quad - \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_{N^{**}-2})) \bar{D}_{2e_1} v(x_{\ell_1}, x_{N^{**}}) \\
&\quad - \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_{N^{**}-1})) \bar{D}_{2e_1} v(x_{\ell_1}, x_{N^{**}+1}) \} \\
&\quad + \frac{\varepsilon^2}{2} \sum_{\ell_1=N^*-1}^{N^{**}-1} \sum_{\ell_2=N^{**}}^N \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_{\ell_2})) \\
&\quad + \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1-2}, x_{\ell_2})) \} \bar{D}_{2e_2} v_\ell \\
&\quad + \frac{\varepsilon^2}{2} \sum_{\ell_2=N^{**}}^N \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^{**}-1}, x_{\ell_2})) \bar{D}_{2e_2} v(x_{N^{**}+1}, x_{\ell_2}) \\
&\quad + \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^{**}-2}, x_{\ell_2})) \bar{D}_{2e_2} v(x_{N^{**}}, x_{\ell_2}) \\
&\quad - \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^*-3}, x_{\ell_2})) \bar{D}_{2e_2} v(x_{N^*-1}, x_{\ell_2}) \\
&\quad - \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^*-2}, x_{\ell_2})) \bar{D}_{2e_2} v(x_{N^*}, x_{\ell_2}) \},
\end{aligned} \tag{5.18}$$



and

$$\begin{aligned}
\langle DE_{\Omega_{a_4}, \eta}^a \{y\}, v \rangle_\varepsilon &= \varepsilon^2 \sum_{\ell_1=N^{**}}^N \sum_{\ell_2=1}^N \nabla_\zeta \phi(\overline{D}_\eta y(x_{\ell_1}, x_{\ell_2})) \overline{D}_\eta v_\ell \\
&= \frac{\varepsilon^2}{2} \sum_{\ell_1=N^{**}}^N \sum_{\ell_2=1}^N \{ \nabla_\zeta \phi(\overline{D}_\eta y(x_{\ell_1}, x_{\ell_2})) + \nabla_\zeta \phi(\overline{D}_\eta y(x_{\ell_1}, x_{\ell_2-2})) \} \overline{D}_{2e_1} v_\ell \\
&\quad + \frac{\varepsilon^2}{2} \sum_{\ell_1=N^{**}}^N \{ \nabla_\zeta \phi(\overline{D}_\eta y(x_{\ell_1}, x_N)) \overline{D}_{2e_1} v(x_{\ell_1}, x_{N+2}) \\
&\quad + \nabla_\zeta \phi(\overline{D}_\eta y(x_{\ell_1}, x_{N-1})) \overline{D}_{2e_1} v(x_{\ell_1}, x_{N+1}) \\
&\quad - \nabla_\zeta \phi(\overline{D}_\eta y(x_{\ell_1}, x_{-1})) \overline{D}_{2e_1} v(x_{\ell_1}, x_1) \\
&\quad - \nabla_\zeta \phi(\overline{D}_\eta y(x_{\ell_1}, x_0)) \overline{D}_{2e_1} v(x_{\ell_1}, x_2) \} \\
&\quad + \frac{\varepsilon^2}{2} \sum_{\ell_1=N^{**}}^N \sum_{\ell_2=1}^N \{ \nabla_\zeta \phi(\overline{D}_\eta y(x_{\ell_1}, x_{\ell_2})) \\
&\quad + \nabla_\zeta \phi(\overline{D}_\eta y(x_{\ell_1-2}, x_{\ell_2})) \} \overline{D}_{2e_2} v_\ell \\
&\quad + \frac{\varepsilon^2}{2} \sum_{\ell_2=1}^N \{ \nabla_\zeta \phi(\overline{D}_\eta y(x_N, x_{\ell_2})) \overline{D}_{2e_2} v(x_{N+2}, x_{\ell_2}) \\
&\quad + \nabla_\zeta \phi(\overline{D}_\eta y(x_{N-1}, x_{\ell_2})) \overline{D}_{2e_2} v(x_{N+1}, x_{\ell_2}) \\
&\quad - \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{\ell_2})) \overline{D}_{2e_2} v(x_{N^{**}+1}, x_{\ell_2}) \\
&\quad - \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-2}, x_{\ell_2})) \overline{D}_{2e_2} v(x_{N^{**}}, x_{\ell_2}) \}.
\end{aligned} \tag{5.19}$$

Now we will add  $\langle DE_{\Omega_{a_1}, \eta}^a \{y\}, v \rangle_\varepsilon$ ,  $\langle DE_{\Omega_{a_2}, \eta}^a \{y\}, v \rangle_\varepsilon$ ,  $\langle DE_{\Omega_{a_3}, \eta}^a \{y\}, v \rangle_\varepsilon$  and  $\langle DE_{\Omega_{a_4}, \eta}^a \{y\}, v \rangle_\varepsilon$  and focus only on the terms that include  $\overline{D}_{2e_2} v_\ell$ , which we will denote as  $H$  as follows on the next page.

$$\begin{aligned}
H = & \frac{\varepsilon^2}{2} \sum_{\ell_1=1}^{N^*-2} \sum_{\ell_2=1}^N \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_{\ell_2})) + \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1-2}, x_{\ell_2})) \} \bar{D}_{2e_2} v_\ell \\
& + \frac{\varepsilon^2}{2} \sum_{\ell_2=1}^N \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^*-2}, x_{\ell_2})) \} \bar{D}_{2e_2} v(x_{N^*}, x_{\ell_2}) \\
& + \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^*-3}, x_{\ell_2})) \bar{D}_{2e_2} v(x_{N^*-1}, x_{\ell_2}) - \nabla_\zeta \phi(\bar{D}_\eta y(x_{-1}, x_{\ell_2})) \bar{D}_{2e_2} v(x_1, x_{\ell_2}) \\
& - \nabla_\zeta \phi(\bar{D}_\eta y(x_0, x_{\ell_2})) \bar{D}_{2e_2} v(x_2, x_{\ell_2}) \} \\
& + \frac{\varepsilon^2}{2} \sum_{\ell_1=N^*-1}^{N^{**}-1} \sum_{\ell_2=1}^{N^*-2} \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_{\ell_2})) + \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1-2}, x_{\ell_2})) \} \bar{D}_{2e_2} v_\ell \\
& + \frac{\varepsilon^2}{2} \sum_{\ell_2=1}^{N^*-2} \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^{**}-1}, x_{\ell_2})) \} \bar{D}_{2e_2} v(x_{N^{**}+1}, x_{\ell_2}) \\
& + \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^{**}-2}, x_{\ell_2})) \bar{D}_{2e_2} v(x_{N^{**}}, x_{\ell_2}) - \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^*-2}, x_{\ell_2})) \bar{D}_{2e_2} v(x_{N^*}, x_{\ell_2}) \\
& - \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^*-3}, x_{\ell_2})) \bar{D}_{2e_2} v(x_{N^*-1}, x_{\ell_2}) \} \\
& + \frac{\varepsilon^2}{2} \sum_{\ell_1=N^*-1}^{N^{**}-1} \sum_{\ell_2=N^{**}}^N \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_{\ell_2})) + \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1-2}, x_{\ell_2})) \} \bar{D}_{2e_2} v_\ell \\
& + \frac{\varepsilon^2}{2} \sum_{\ell_2=N^{**}}^N \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^{**}-1}, x_{\ell_2})) \} \bar{D}_{2e_2} v(x_{N^{**}+1}, x_{\ell_2}) \\
& + \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^{**}-2}, x_{\ell_2})) \bar{D}_{2e_2} v(x_{N^{**}}, x_{\ell_2}) - \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^*-3}, x_{\ell_2})) \bar{D}_{2e_2} v(x_{N^*-1}, x_{\ell_2}) \\
& - \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^*-2}, x_{\ell_2})) \bar{D}_{2e_2} v(x_{N^*}, x_{\ell_2}) \} \\
& + \frac{\varepsilon^2}{2} \sum_{\ell_1=N^{**}}^N \sum_{\ell_2=1}^N \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_{\ell_2})) + \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1-2}, x_{\ell_2})) \} \bar{D}_{2e_2} v_\ell \\
& + \frac{\varepsilon^2}{2} \sum_{\ell_2=1}^N \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_N, x_{\ell_2})) \} \bar{D}_{2e_2} v(x_{N+2}, x_{\ell_2}) \\
& + \nabla_\zeta \phi(\bar{D}_\eta y(x_{N-1}, x_{\ell_2})) \bar{D}_{2e_2} v(x_{N+1}, x_{\ell_2}) - \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^{**}-1}, x_{\ell_2})) \bar{D}_{2e_2} v(x_{N^{**}+1}, x_{\ell_2}) \\
& - \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^{**}-2}, x_{\ell_2})) \bar{D}_{2e_2} v(x_{N^{**}}, x_{\ell_2}) \}.
\end{aligned} \tag{5.20}$$

We can simplify  $H$  by applying the periodicity conditions

$$\phi(\bar{D}_\eta y(x_N, x_{\ell_2})) \bar{D}_{2e_2} v(x_{N+2}, x_{\ell_2}) = \phi(\bar{D}_\eta y(x_0, x_{\ell_2})) \bar{D}_{2e_2} v(x_2, x_{\ell_2}), \tag{5.21}$$

and

$$\phi(\bar{D}_\eta y(x_{N-1}, x_{\ell_2})) \bar{D}_{2e_2} v(x_{N+1}, x_{\ell_2}) = \phi(\bar{D}_\eta y(x_{-1}, x_{\ell_2})) \bar{D}_{2e_2} v(x_1, x_{\ell_2}), \tag{5.22}$$

to (5.20) and hence some terms cancel out and we obtain

$$\begin{aligned}
H = & \frac{\varepsilon^2}{2} \sum_{\ell_1=1}^{N^*-2} \sum_{\ell_2=1}^N \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_{\ell_2})) + \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1-2}, x_{\ell_2})) \} \bar{D}_{2e_2} v_\ell \\
& + \frac{\varepsilon^2}{2} \sum_{\ell_2=N^*-1}^{N^{**}-1} \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^*-2}, x_{\ell_2})) \} \bar{D}_{2e_2} v(x_{N^*}, x_{\ell_2}) \\
& + \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^*-3}, x_{\ell_2})) \bar{D}_{2e_2} v(x_{N^*-1}, x_{\ell_2}) \\
& + \frac{\varepsilon^2}{2} \sum_{\ell_1=N^*-1}^{N^{**}-1} \sum_{\ell_2=1}^{N^*-2} \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_{\ell_2})) + \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1-2}, x_{\ell_2})) \} \bar{D}_{2e_2} v_\ell \\
& + \frac{\varepsilon^2}{2} \sum_{\ell_1=N^*-1}^{N^{**}-1} \sum_{\ell_2=N^{**}}^N \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_{\ell_2})) + \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1-2}, x_{\ell_2})) \} \bar{D}_{2e_2} v_\ell \\
& + \frac{\varepsilon^2}{2} \sum_{\ell_1=N^{**}}^N \sum_{\ell_2=1}^N \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_{\ell_2})) + \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1-2}, x_{\ell_2})) \} \bar{D}_{2e_2} v_\ell \\
& - \frac{\varepsilon^2}{2} \sum_{\ell_2=N^*-1}^{N^{**}-1} \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^{**}-1}, x_{\ell_2})) \} \bar{D}_{2e_2} v(x_{N^{**}+1}, x_{\ell_2}) \\
& + \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^{**}-2}, x_{\ell_2})) \bar{D}_{2e_2} v(x_{N^{**}}, x_{\ell_2}) \}.
\end{aligned} \tag{5.23}$$

We have to further reduce the above in terms of  $\bar{D}_{e_2} v_\ell$  by using the splitting

$$\bar{D}_{2e_2} v_\ell = \bar{D}_{e_2} v_\ell + \bar{D}_{e_2} v_{\ell+e_2}, \tag{5.24}$$

as follows

$$\begin{aligned}
H = & \frac{\varepsilon^2}{2} \sum_{\ell_1=1}^{N^*-2} \sum_{\ell_2=1}^N \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_{\ell_2})) + \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1-2}, x_{\ell_2})) \} [\bar{D}_{e_2} v_\ell + \bar{D}_{e_2} v_{\ell+e_2}] \\
& + \frac{\varepsilon^2}{2} \sum_{\ell_1=N^*-1}^{N^{**}-1} \sum_{\ell_2=1}^{N^*-2} \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_{\ell_2})) + \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1-2}, x_{\ell_2})) \} [\bar{D}_{e_2} v_\ell \\
& + \bar{D}_{e_2} v_{\ell+e_2}] + \frac{\varepsilon^2}{2} \sum_{\ell_1=N^*-1}^{N^{**}-1} \sum_{\ell_2=N^{**}}^N \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_{\ell_2})) + \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1-2}, x_{\ell_2})) \} \\
& [\bar{D}_{e_2} v_\ell + \bar{D}_{e_2} v_{\ell+e_2}] + \frac{\varepsilon^2}{2} \sum_{\ell_1=N^{**}}^N \sum_{\ell_2=1}^N \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_{\ell_2})) + \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1-2}, x_{\ell_2})) \} \\
& [\bar{D}_{e_2} v_\ell + \bar{D}_{e_2} v_{\ell+e_2}] + \frac{\varepsilon^2}{2} \sum_{\ell_2=N^*-1}^{N^{**}-1} \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^*-2}, x_{\ell_2})) \} [\bar{D}_{e_2} v(x_{N^*}, x_{\ell_2}) \\
& + \bar{D}_{e_2} v(x_{N^*}, x_{\ell_2+1})] + \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^*-3}, x_{\ell_2})) [\bar{D}_{e_2} v(x_{N^*-1}, x_{\ell_2}) \\
& + \bar{D}_{e_2} v(x_{N^*-1}, x_{\ell_2+1})] \} - \frac{\varepsilon^2}{2} \sum_{\ell_2=N^*-1}^{N^{**}-1} \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^{**}-1}, x_{\ell_2})) \} [\bar{D}_{e_2} v(x_{N^{**}+1}, x_{\ell_2}) \\
& + \bar{D}_{e_2} v(x_{N^{**}+1}, x_{\ell_2+1})] + \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^{**}-2}, x_{\ell_2})) [\bar{D}_{e_2} v(x_{N^{**}}, x_{\ell_2}) \\
& + \bar{D}_{e_2} v(x_{N^{**}}, x_{\ell_2+1})] \}.
\end{aligned} \tag{5.25}$$

Finally, we change the indexing where necessary to convert all the terms to be of the form  $\bar{D}_{e_2} v_\ell$ , which yields

$$\begin{aligned}
H = & \frac{\varepsilon^2}{2} \sum_{\ell_1=1}^{N^*-2} \sum_{\ell_2=1}^N \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_{\ell_2})) + \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1-2}, x_{\ell_2})) \} \bar{D}_{e_2} v_\ell \\
& + \frac{\varepsilon^2}{2} \sum_{\ell_1=1}^{N^*-2} \sum_{\ell_2=2}^{N+1} \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_{\ell_2-1})) + \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1-2}, x_{\ell_2-1})) \} \bar{D}_{e_2} v_\ell \\
& + \frac{\varepsilon^2}{2} \sum_{\ell_1=N^*-1}^{N^{**}-1} \sum_{\ell_2=1}^{N^*-2} \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_{\ell_2})) + \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1-2}, x_{\ell_2})) \} \bar{D}_{e_2} v_\ell \\
& + \frac{\varepsilon^2}{2} \sum_{\ell_1=N^*-1}^{N^{**}-1} \sum_{\ell_2=2}^{N^*-1} \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_{\ell_2-1})) + \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1-2}, x_{\ell_2-1})) \} \bar{D}_{e_2} v_\ell \\
& + \frac{\varepsilon^2}{2} \sum_{\ell_1=N^*-1}^{N^{**}-1} \sum_{\ell_2=N^{**}}^N \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_{\ell_2})) + \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1-2}, x_{\ell_2})) \} \bar{D}_{e_2} v_\ell \\
& + \frac{\varepsilon^2}{2} \sum_{\ell_1=N^*-1}^{N^{**}-1} \sum_{\ell_2=N^{**}+1}^{N+1} \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_{\ell_2-1})) + \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1-2}, x_{\ell_2-1})) \} \bar{D}_{e_2} v_\ell \\
& + \frac{\varepsilon^2}{2} \sum_{\ell_1=N^{**}}^N \sum_{\ell_2=1}^N \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_{\ell_2})) + \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1-2}, x_{\ell_2})) \} \bar{D}_{e_2} v_\ell \\
& + \frac{\varepsilon^2}{2} \sum_{\ell_1=N^{**}}^N \sum_{\ell_2=2}^{N+1} \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_{\ell_2-1})) + \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1-2}, x_{\ell_2-1})) \} \bar{D}_{e_2} v_\ell \\
& + \frac{\varepsilon^2}{2} \sum_{\ell_2=N^*-1}^{N^{**}-1} \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^*-2}, x_{\ell_2})) \bar{D}_{e_2} v(x_{N^*}, x_{\ell_2}) \\
& + \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^*-3}, x_{\ell_2})) \bar{D}_{e_2} v(x_{N^*-1}, x_{\ell_2}) \} \\
& + \frac{\varepsilon^2}{2} \sum_{\ell_2=N^*}^{N^{**}} \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^*-2}, x_{\ell_2-1})) \bar{D}_{e_2} v(x_{N^*}, x_{\ell_2}) \\
& + \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^*-3}, x_{\ell_2-1})) \bar{D}_{e_2} v(x_{N^*-1}, x_{\ell_2}) \} \\
& - \frac{\varepsilon^2}{2} \sum_{\ell_2=N^*-1}^{N^{**}-1} \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^{**}-1}, x_{\ell_2})) \bar{D}_{e_2} v(x_{N^{**}+1}, x_{\ell_2}) \\
& + \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^{**}-2}, x_{\ell_2})) \bar{D}_{e_2} v(x_{N^{**}}, x_{\ell_2}) \} \\
& - \frac{\varepsilon^2}{2} \sum_{\ell_2=N^*}^{N^{**}} \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^{**}-1}, x_{\ell_2-1})) \bar{D}_{e_2} v(x_{N^{**}+1}, x_{\ell_2}) \\
& + \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^{**}-2}, x_{\ell_2-1})) \bar{D}_{e_2} v(x_{N^{**}}, x_{\ell_2+1}) \}.
\end{aligned} \tag{5.26}$$

Now we will rewrite the double sums into their original forms as in (5.10)

$$\begin{aligned}
H = & \frac{\varepsilon^2}{2} \sum_{\ell_1=1}^{N^*-1} \sum_{\ell_2=1}^N \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_{\ell_2})) + \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1-2}, x_{\ell_2})) \} \bar{D}_{e_2} v_\ell \\
& + \frac{\varepsilon^2}{2} \sum_{\ell_1=1}^{N^*-1} \sum_{\ell_2=1}^N \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_{\ell_2-1})) + \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1-2}, x_{\ell_2-1})) \} \bar{D}_{e_2} v_\ell \\
& + \frac{\varepsilon^2}{2} \sum_{\ell_1=N^*}^{N^{**}-1} \sum_{\ell_2=1}^{N^*-1} \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_{\ell_2-1})) + \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1-2}, x_{\ell_2-1})) \} \bar{D}_{e_2} v_\ell \\
& + \frac{\varepsilon^2}{2} \sum_{\ell_1=N^*}^{N^{**}-1} \sum_{\ell_2=1}^{N^*-1} \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_{\ell_2})) + \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1-2}, x_{\ell_2})) \} \bar{D}_{e_2} v_\ell \\
& + \frac{\varepsilon^2}{2} \sum_{\ell_1=N^*}^{N^{**}-1} \sum_{\ell_2=N^{**}}^N \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_{\ell_2})) + \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1-2}, x_{\ell_2})) \} \bar{D}_{e_2} v_\ell \\
& + \frac{\varepsilon^2}{2} \sum_{\ell_1=N^*}^{N^{**}-1} \sum_{\ell_2=N^{**}}^N \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_{\ell_2-1})) + \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1-2}, x_{\ell_2-1})) \} \bar{D}_{e_2} v_\ell \\
& + \frac{\varepsilon^2}{2} \sum_{\ell_1=N^{**}}^N \sum_{\ell_2=1}^N \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_{\ell_2})) + \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1-2}, x_{\ell_2})) \} \bar{D}_{e_2} v_\ell \\
& + \frac{\varepsilon^2}{2} \sum_{\ell_1=N^{**}}^N \sum_{\ell_2=1}^N \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_{\ell_2-1})) + \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1-2}, x_{\ell_2-1})) \} \bar{D}_{e_2} v_\ell \\
& - \frac{\varepsilon^2}{2} \sum_{\ell_2=1}^N \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^*-1}, x_{\ell_2})) + \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^*-3}, x_{\ell_2})) \} \bar{D}_{e_2} v(x_{N^*-1}, x_{\ell_2}) \\
& + \frac{\varepsilon^2}{2} \sum_{\ell_1=1}^{N^*-2} \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_N)) + \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1-2}, x_N)) \} \bar{D}_{e_2} v(x_{\ell_1}, x_{N+1}) \\
& - \frac{\varepsilon^2}{2} \sum_{\ell_1=1}^{N^*-2} \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_0)) + \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1-2}, x_0)) \} \bar{D}_{e_2} v(x_{\ell_1}, x_1) \\
& - \frac{\varepsilon^2}{2} \sum_{\ell_2=1}^N \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^*-1}, x_{\ell_2-1})) + \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^*-3}, x_{\ell_2-1})) \} \bar{D}_{e_2} v(x_{N^*-1}, x_{\ell_2}) \\
& + \frac{\varepsilon^2}{2} \sum_{\ell_2=1}^{N^*-1} \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^*-1}, x_{\ell_2-1})) + \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^*-3}, x_{\ell_2-1})) \} \bar{D}_{e_2} v(x_{N^*-1}, x_{\ell_2}) \\
& - \frac{\varepsilon^2}{2} \sum_{\ell_1=N^*-1}^{N^{**}-1} \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_0)) + \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1-2}, x_0)) \} \bar{D}_{e_2} v(x_{\ell_1}, x_1) \\
& + \frac{\varepsilon^2}{2} \sum_{\ell_2=1}^{N^*-1} \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^*-1}, x_{\ell_2})) + \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^*-3}, x_{\ell_2})) \} \bar{D}_{e_2} v(x_{N^*-1}, x_{\ell_2}) \\
& - \frac{\varepsilon^2}{2} \sum_{\ell_1=N^*-1}^{N^{**}-1} \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_{N^*-1})) \}
\end{aligned} \tag{5.27}$$

$$\begin{aligned}
& + \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1-2}, x_{N^*-1})) \bar{D}_{e_2} v(x_{\ell_1}, x_{N^*-1}) \\
& + \frac{\varepsilon^2}{2} \sum_{\ell_2=N^{**}}^N \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^*-1}, x_{\ell_2})) + \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^*-3}, x_{\ell_2})) \} \bar{D}_{e_2} v(x_{N^*-1}, x_{\ell_2}) \\
& + \frac{\varepsilon^2}{2} \sum_{\ell_1=N^*-1}^{N^{**}-1} \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_N)) + \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1-2}, x_N)) \} \bar{D}_{e_2} v(x_{\ell_1}, x_{N+1}) \\
& - \frac{\varepsilon^2}{2} \sum_{\ell_1=N^*-1}^{N^{**}-1} \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_{N^{**}-1})) + \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1-2}, x_{N^{**}-1})) \} \bar{D}_{e_2} v(x_{\ell_1}, x_{N^{**}}) \\
& + \frac{\varepsilon^2}{2} \sum_{\ell_2=N^{**}}^N \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^*-1}, x_{\ell_2-1})) + \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^*-3}, x_{\ell_2-1})) \} \bar{D}_{e_2} v(x_{N^*-1}, x_{\ell_2}) \\
& + \frac{\varepsilon^2}{2} \sum_{\ell_1=N^{**}}^N \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_N)) + \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1-2}, x_N)) \} \bar{D}_{e_2} v(x_{\ell_1}, x_{N+1}) \\
& - \frac{\varepsilon^2}{2} \sum_{\ell_1=N^{**}}^N \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_0)) + \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1-2}, x_0)) \} \bar{D}_{e_2} v(x_{\ell_1}, x_1) \\
& + \frac{\varepsilon^2}{2} \sum_{\ell_2=N^*-1}^{N^{**}-1} \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^*-2}, x_{\ell_2})) \} \bar{D}_{e_2} v(x_{N^*}, x_{\ell_2}) \\
& + \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^*-3}, x_{\ell_2})) \bar{D}_{e_2} v(x_{N^*-1}, x_{\ell_2}) \\
& + \frac{\varepsilon^2}{2} \sum_{\ell_2=N^*}^{N^{**}} \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^*-2}, x_{\ell_2-1})) \} \bar{D}_{e_2} v(x_{N^*}, x_{\ell_2}) \\
& + \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^*-3}, x_{\ell_2-1})) \bar{D}_{e_2} v(x_{N^*-1}, x_{\ell_2}) \} \\
& - \frac{\varepsilon^2}{2} \sum_{\ell_2=N^*-1}^{N^{**}-1} \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^{**}-1}, x_{\ell_2})) \} \bar{D}_{e_2} v(x_{N^{**}+1}, x_{\ell_2}) \\
& + \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^{**}-2}, x_{\ell_2})) \bar{D}_{e_2} v(x_{N^{**}}, x_{\ell_2}) \} \\
& - \frac{\varepsilon^2}{2} \sum_{\ell_2=N^*}^{N^{**}} \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^{**}-1}, x_{\ell_2-1})) \} \bar{D}_{e_2} v(x_{N^{**}+1}, x_{\ell_2}) \\
& + \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^{**}-2}, x_{\ell_2-1})) \bar{D}_{e_2} v(x_{N^{**}}, x_{\ell_2}) \}.
\end{aligned} \tag{5.28}$$

Some terms cancel out due to periodicity and after some further simplifications we obtain

$$\begin{aligned}
H = & \frac{\varepsilon^2}{2} \sum_{\ell_1=1}^{N^*-1} \sum_{\ell_2=1}^N \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_{\ell_2})) + \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1-2}, x_{\ell_2})) \\
& + \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_{\ell_2-1})) + \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1-2}, x_{\ell_2-1})) \} \bar{D}_{e_2} v_\ell \\
& + \frac{\varepsilon^2}{2} \sum_{\ell_1=N^*}^{N^{**}-1} \sum_{\ell_2=1}^{N^*-1} \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_{\ell_2})) + \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1-2}, x_{\ell_2})) \\
& + \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_{\ell_2-1})) + \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1-2}, x_{\ell_2-1})) \} \bar{D}_{e_2} v_\ell \\
& + \frac{\varepsilon^2}{2} \sum_{\ell_1=N^*}^{N^{**}-1} \sum_{\ell_2=N^{**}}^N \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_{\ell_2})) + \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1-2}, x_{\ell_2})) \\
& + \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_{\ell_2-1})) + \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1-2}, x_{\ell_2-1})) \} \bar{D}_{e_2} v_\ell \\
& + \frac{\varepsilon^2}{2} \sum_{\ell_1=N^{**}}^N \sum_{\ell_2=1}^N \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_{\ell_2})) + \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1-2}, x_{\ell_2})) \\
& + \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_{\ell_2-1})) + \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1-2}, x_{\ell_2-1})) \} \bar{D}_{e_2} v_\ell \\
& - \frac{\varepsilon^2}{2} \sum_{\ell_2=N^*}^{N^{**}-1} \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^*-1}, x_{\ell_2})) + \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^*-3}, x_{\ell_2})) \} \bar{D}_{e_2} v(x_{N^*-1}, x_{\ell_2}) \\
& - \frac{\varepsilon^2}{2} \sum_{\ell_2=N^*}^{N^{**}-1} \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^*-1}, x_{\ell_2-1})) \\
& + \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^*-3}, x_{\ell_2-1})) \} \bar{D}_{e_2} v(x_{N^*-1}, x_{\ell_2}) \\
& - \frac{\varepsilon^2}{2} \sum_{\ell_1=N^*-1}^{N^{**}-1} \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_{N^*-1})) \\
& + \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1-2}, x_{N^*-1})) \} \bar{D}_{e_2} v(x_{\ell_1}, x_{N^*-1}) \\
& - \frac{\varepsilon^2}{2} \sum_{\ell_1=N^*-1}^{N^{**}-1} \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_{N^{**}-1})) \\
& + \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1-2}, x_{N^{**}-1})) \} \bar{D}_{e_2} v(x_{\ell_1}, x_{N^{**}}) \\
& + \frac{\varepsilon^2}{2} \sum_{\ell_2=N^*-1}^{N^{**}-1} \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^*-2}, x_{\ell_2})) \} \bar{D}_{e_2} v(x_{N^*}, x_{\ell_2}) \\
& + \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^*-3}, x_{\ell_2})) \bar{D}_{e_2} v(x_{N^*-1}, x_{\ell_2}) \\
& + \frac{\varepsilon^2}{2} \sum_{\ell_2=N^*}^{N^{**}} \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^*-2}, x_{\ell_2-1})) \} \bar{D}_{e_2} v(x_{N^*}, x_{\ell_2}) \\
& + \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^*-3}, x_{\ell_2-1})) \bar{D}_{e_2} v(x_{N^*-1}, x_{\ell_2}) \} \\
& - \frac{\varepsilon^2}{2} \sum_{\ell_2=N^*-1}^{N^{**}-1} \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^{**}-1}, x_{\ell_2})) \} \bar{D}_{e_2} v(x_{N^{**}+1}, x_{\ell_2}) \\
& + \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^{**}-2}, x_{\ell_2})) \bar{D}_{e_2} v(x_{N^{**}}, x_{\ell_2}) \}
\end{aligned}$$

$$\begin{aligned}
& -\frac{\varepsilon^2}{2} \sum_{\ell_2=N^*}^{N^{**}} \{ \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{\ell_2-1})) \overline{D}_{e_2} v(x_{N^{**}+1}, x_{\ell_2}) \\
& + \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-2}, x_{\ell_2-1})) \overline{D}_{e_2} v(x_{N^{**}}, x_{\ell_2}) \}.
\end{aligned} \tag{5.29}$$

The double sums are treated by using the following lemma

**Lemma 23.** *For smooth functions  $y$  and  $\phi$  we have*

$$\begin{aligned}
& 2\nabla_\zeta \phi(\nabla y(m_{(\ell_1, \ell_2)})\eta) + 2\nabla_\zeta \phi(\nabla y(m_{(\ell_1-1, \ell_2)})\eta) - \nabla_\zeta \phi(\overline{D}_\eta y(x_{\ell_1}, x_{\ell_2})) \\
& - \nabla_\zeta \phi(\overline{D}_\eta y(x_{\ell_1-2}, x_{\ell_2})) - \nabla_\zeta \phi(\overline{D}_\eta y(x_{\ell_1}, x_{\ell_2-1})) - \nabla_\zeta \phi(\overline{D}_\eta y(x_{\ell_1-2}, x_{\ell_2-1})) \leq O(\varepsilon^2).
\end{aligned} \tag{5.30}$$

*Proof.* See the proof of Lemma 3.1 in [21].  $\square$

Now we subtract H from  $Z$  and we apply Lemma 23 and so some of the terms are of order  $O(\varepsilon^2)$ . We set  $W$  to be the sum of the remaining terms that we need to examine such that

$$\begin{aligned}
W = & \varepsilon^2 \sum_{\ell_2=N^*}^{N^{**}-1} \nabla_\zeta \phi(\nabla y(m_{N^*-1, \ell_2})\eta) \overline{D}_{e_2} v(x_{N^*}, x_{\ell_2}) \\
& - \varepsilon^2 \sum_{\ell_2=N^*}^{N^{**}-1} \nabla_\zeta \phi(\nabla y(m_{N^{**}-1, \ell_2})\eta) \overline{D}_{e_2} v(x_{N^{**}}, x_{\ell_2}) \\
& + \frac{\varepsilon^2}{2} \sum_{\ell_2=N^*}^{N^{**}-1} \{ \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^*-1}, x_{\ell_2})) \\
& + \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^*-3}, x_{\ell_2})) \} \overline{D}_{e_2} v(x_{N^*-1}, x_{\ell_2}) \\
& + \frac{\varepsilon^2}{2} \sum_{\ell_2=N^*}^{N^{**}-1} \{ \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^*-1}, x_{\ell_2-1})) \\
& + \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^*-3}, x_{\ell_2-1})) \} \overline{D}_{e_2} v(x_{N^*-1}, x_{\ell_2}) \\
& + \frac{\varepsilon^2}{2} \sum_{\ell_1=N^*-1}^{N^{**}-1} \{ \nabla_\zeta \phi(\overline{D}_\eta y(x_{\ell_1}, x_{N^*-1})) \\
& + \nabla_\zeta \phi(\overline{D}_\eta y(x_{\ell_1-2}, x_{N^*-1})) \} \overline{D}_{e_2} v(x_{\ell_1}, x_{N^*-1}) \\
& + \frac{\varepsilon^2}{2} \sum_{\ell_1=N^*-1}^{N^{**}-1} \{ \nabla_\zeta \phi(\overline{D}_\eta y(x_{\ell_1}, x_{N^{**}-1})) \\
& + \nabla_\zeta \phi(\overline{D}_\eta y(x_{\ell_1-2}, x_{N^{**}-1})) \} \overline{D}_{e_2} v(x_{\ell_1}, x_{N^{**}}) \\
& - \frac{\varepsilon^2}{2} \sum_{\ell_2=N^*-1}^{N^{**}-1} \{ \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^*-2}, x_{\ell_2})) \overline{D}_{e_2} v(x_{N^*}, x_{\ell_2}) \\
& + \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^*-3}, x_{\ell_2})) \overline{D}_{e_2} v(x_{N^*-1}, x_{\ell_2}) \}
\end{aligned}$$



$$\begin{aligned}
& -\frac{\varepsilon^2}{2} \sum_{\ell_2=N^*}^{N^{**}} \{ \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^*-2}, x_{\ell_2-1})) \overline{D}_{e_2} v(x_{N^*}, x_{\ell_2}) \\
& + \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^*-3}, x_{\ell_2-1})) \overline{D}_{e_2} v(x_{N^*-1}, x_{\ell_2}) \} \\
& + \frac{\varepsilon^2}{2} \sum_{\ell_2=N^*-1}^{N^{**}-1} \{ \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{\ell_2})) \overline{D}_{e_2} v(x_{N^{**}+1}, x_{\ell_2}) \\
& + \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-2}, x_{\ell_2})) \overline{D}_{e_2} v(x_{N^{**}}, x_{\ell_2}) \} \\
& + \frac{\varepsilon^2}{2} \sum_{\ell_2=N^*}^{N^{**}} \{ \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{\ell_2-1})) \overline{D}_{e_2} v(x_{N^{**}+1}, x_{\ell_2}) \\
& + \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-2}, x_{\ell_2-1})) \overline{D}_{e_2} v(x_{N^{**}}, x_{\ell_2}) \}.
\end{aligned} \tag{5.31}$$

We still need to subtract the first variation of the bond volumes that intersect the interfaces,  $\langle DE_{\Gamma, \eta}^D, v \rangle_\varepsilon = \langle DE_{\Gamma_1, \eta}, v \rangle_\varepsilon + \langle DE_{\Gamma_2, \eta}, v \rangle_\varepsilon + \langle DE_{\Gamma_3, \eta}, v \rangle_\varepsilon + \langle DE_{\Gamma_4, \eta}, v \rangle_\varepsilon$ . In the next section we compute these first variations.

### 5.2.1 The First Variation of the Interface Terms

Recall from Chapter 1, (1.40) that the energy on the interface is

$$\begin{aligned}
E_{\Gamma, \eta}^D \{y\} &= \sum_{\substack{\ell \in \mathcal{L} \\ B_{\ell, \eta} \in B_\Gamma}} \frac{1}{|\eta_1 \eta_2|} \left[ \int_{B_{\ell, \eta}} \chi_{\Omega_a} \phi(\nabla y^{\ell, \eta}) dx - \int_{B_{\ell, \eta} \cap \Gamma} \phi'(\{\nabla y^{\ell, \eta}\}) \cdot [y^{\ell, \eta}] dS \right] \\
&=: E_1 + E_2.
\end{aligned} \tag{5.32}$$

The energy on the interface (5.32) was used in the one dimensional case in Chapters 2 and 3. As explained in Section 4.4, in the two dimensional case this energy on the interface had to be altered. In the  $E_1$  term, we replaced  $\phi(\nabla y^{\ell, \eta})$  with  $\phi(\overline{D}_\eta y_\ell)$  and the  $E_2$  term takes a different form due to the analysis in this chapter and will be explained further in Section 5.2.2 and 5.2.3. We will focus first on the  $E_1$  terms. In Section 4.6, Chapter 4, we had stated the energy on each interface and corners. The energy on interface  $\Gamma_1$  for the term that represents  $E_1$  is

$$E_{1, \Gamma_1} \{y\} = \sum_{\ell_1=N^*}^{N^{**}-2} \frac{1}{4} \int_{B_{(\ell_1, N^{**}-1), \eta}} \chi_{\Omega_a} \phi(\overline{D}_\eta y_\ell) dx. \tag{5.33}$$

The first variation of this interface is:

$$\langle DE_{1, \Gamma_1}, v \rangle_\varepsilon = \frac{\varepsilon^2}{2} \sum_{\ell_1=N^*}^{N^{**}-2} \nabla_\zeta \phi(\overline{D}_\eta y(x_{\ell_1}, x_{N^{**}-1})) \overline{D}_\eta v(x_{\ell_1}, x_{N^{**}-1}). \tag{5.34}$$

which is the first term in (4.72). Similarly, the first variation of the energy on interface  $\Gamma_2$  for the term that represents  $E_2$  is

$$\langle DE_{1, \Gamma_2}, v \rangle_\varepsilon = \frac{\varepsilon^2}{2} \sum_{\ell_2=N^*}^{N^{**}-2} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{\ell_2})) \overline{D}_\eta v(x_{N^{**}-1}, x_{\ell_2}), \tag{5.35}$$

the first variation of the energy on interface  $\Gamma_3$  for the term that represents  $E_3$  is

$$\langle DE_{1,\Gamma_3}, v \rangle_\varepsilon = \frac{\varepsilon^2}{2} \sum_{\ell_1 N^{*-1}}^{N^{**}-2} \nabla_\zeta \phi(\overline{D}_\eta y(x_{\ell_1}, x_{N^{*-1}})) \overline{D}_\eta v(x_{\ell_1}, x_{N^{*-1}}), \quad (5.36)$$

and finally, the first variation of the energy on interface  $\Gamma_4$  for the term that represents  $E_4$  is

$$\langle DE_{1,\Gamma_4}, v \rangle_\varepsilon = \frac{\varepsilon^2}{2} \sum_{\ell_2=N^*}^{N^{**}-2} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{*-1}}, x_{\ell_2})) \overline{D}_\eta v(x_{N^{*-1}}, x_{\ell_2}). \quad (5.37)$$

The energy on the corner  $C_1$  for the term that represents  $E_1$  is

$$E_{C_1}\{y\} = \frac{1}{4} \int_{B(N^{*-1}, N^{**}-1), \eta} \chi_{\Omega_a} \phi(\overline{D}_\eta y_\ell) dx.$$

The first variation of the energy on this corner is,

$$\langle DE_{1,C_1}, v \rangle_\varepsilon = \frac{3\varepsilon^2}{4} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{*-1}}, x_{N^{**}-1})) \overline{D}_\eta v(x_{N^{*-1}}, x_{N^{**}-1}). \quad (5.38)$$

Similarly, the first variation of the energy on the corner  $C_2$  for the term that represents  $E_1$  is,

$$\langle DE_{1,C_2}, v \rangle_\varepsilon = \frac{3\varepsilon^2}{4} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{N^{*-1}})) \overline{D}_\eta v(x_{N^{**}-1}, x_{N^{*-1}}), \quad (5.39)$$

the first variation of the energy on the corner  $C_3$  for the term that represents  $E_1$  is,

$$\langle DE_{1,C_3}, v \rangle_\varepsilon = \frac{3\varepsilon^2}{4} \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{N^{*-1}})) \overline{D}_\eta v(x_{N^{**}-1}, x_{N^{*-1}}), \quad (5.40)$$

and finally, the first variation of the energy on the corner  $C_4$  for the term that represents  $E_1$  is

$$\langle DE_{1,C_4}, v \rangle_\varepsilon = \frac{3\varepsilon^2}{4} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{*-1}}, x_{N^{*-1}})) \overline{D}_\eta v(x_{N^{*-1}}, x_{N^{*-1}}). \quad (5.41)$$

We will focus only on the variation of the  $\Gamma_1$  interface energy and apply the same steps to the variation of the other interfaces and corners. The aim is to express the variation of the  $\Gamma_1$  interface energy in terms of  $\overline{D}_{e_2} v_\ell$ , as we did similarly in (5.10). First, we substitute the splitting

$$\begin{aligned} \overline{D}_\eta v(x_{\ell_1}, x_{N^{**}-1}) &= \frac{1}{2} \{ \overline{D}_{2e_1} v(x_{\ell_1}, x_{N^{**}-1}) + \overline{D}_{2e_1} v(x_{\ell_1}, x_{N^{**}+1}) \} \\ &\quad + \frac{1}{2} \{ \overline{D}_{2e_2} v(x_{\ell_1}, x_{N^{**}-1}) + \overline{D}_{2e_2} v(x_{\ell_1+2}, x_{N^{**}-1}) \}, \end{aligned} \quad (5.42)$$

into the first variation of the interface energy  $\Gamma_1$  as follows

$$\begin{aligned} \langle DE_{1,\Gamma_1}\{y\}, v \rangle_\varepsilon &= \sum_{\ell_1=N^*}^{N^{**}-2} \frac{2\varepsilon^2}{4} \nabla_\zeta \phi(\overline{D}_\eta y(x_{\ell_1}, x_{N^{**}-1})) \left[ \frac{1}{2} \{ \overline{D}_{2e_1} v(x_{\ell_1}, x_{N^{**}-1}) \right. \\ &\quad \left. + \overline{D}_{2e_1} v(x_{\ell_1}, x_{N^{**}+1}) \} + \frac{1}{2} \{ \overline{D}_{2e_2} v(x_{\ell_1}, x_{N^{**}-1}) + \overline{D}_{2e_2} v(x_{\ell_1+2}, x_{N^{**}-1}) \} \right]. \end{aligned} \quad (5.43)$$

Then we focus on the terms in the  $e_2$  direction and we change the index for the  $\overline{D}_{2e_2}v(x_{\ell_1+2}, x_{N^{**}-1})$  term from  $\ell_1$  to  $\ell'_1 = \ell_1 + 2$  and we will drop the apostrophe for simplicity. Denote by  $\langle \cdot, \cdot \rangle_{e_2}$  the terms in the  $e_2$  direction of  $\langle \cdot, \cdot \rangle_\varepsilon$ . We use the splitting

$$\overline{D}_{2e_2}v(x_{\ell_1}, x_{N^{**}-1}) = \overline{D}_{e_2}v(x_{\ell_1}, x_{N^{**}-1}) + \overline{D}_{e_2}v(x_{\ell_1}, x_{N^{**}}), \quad (5.44)$$

to obtain

$$\begin{aligned} \langle DE_{1,\Gamma_1}, v \rangle_{e_2} &= \sum_{\ell_1=N^*}^{N^{**}-2} \frac{2\varepsilon^2}{4} \nabla_\zeta \phi(\overline{D}_\eta y(x_{\ell_1}, x_{N^{**}-1})) \left\{ \frac{1}{2} \overline{D}_{2e_2}v(x_{\ell_1}, x_{N^{**}-1}) \right. \\ &\quad \left. + \frac{1}{2} \overline{D}_{2e_2}v(x_{\ell_1+2}, x_{N^{**}-1}) \right\} \\ &= \frac{\varepsilon^2}{4} \sum_{\ell_1=N^*}^{N^{**}-2} \nabla_\zeta \phi(\overline{D}_\eta y(x_{\ell_1}, x_{N^{**}-1})) \overline{D}_{2e_2}v(x_{\ell_1}, x_{N^{**}-1}) \\ &\quad + \frac{\varepsilon^2}{4} \sum_{\ell_1=N^*+2}^{N^{**}} \nabla_\zeta \phi(\overline{D}_\eta y(x_{\ell_1-2}, x_{N^{**}-1})) \overline{D}_{2e_2}v(x_{\ell_1}, x_{N^{**}-1}) \\ &= \frac{\varepsilon^2}{4} \sum_{\ell_1=N^*}^{N^{**}-2} \nabla_\zeta \phi(\overline{D}_\eta y(x_{\ell_1}, x_{N^{**}-1})) \{ \overline{D}_{e_2}v(x_{\ell_1}, x_{N^{**}-1}) + \overline{D}_{e_2}v(x_{\ell_1}, x_{N^{**}}) \} \\ &\quad + \frac{\varepsilon^2}{4} \sum_{\ell_1=N^*+2}^{N^{**}} \nabla_\zeta \phi(\overline{D}_\eta y(x_{\ell_1-2}, x_{N^{**}-1})) \{ \overline{D}_{e_2}v(x_{\ell_1}, x_{N^{**}-1}) \\ &\quad + \overline{D}_{e_2}v(x_{\ell_1}, x_{N^{**}}) \}, \end{aligned} \quad (5.45)$$

Similarly, the first variation of the interface energy  $\Gamma_2$  is:

$$\begin{aligned} \langle DE_{1,\Gamma_2}, v \rangle_{e_2} &= \frac{\varepsilon^2}{4} \sum_{\ell_2=N^*}^{N^{**}-2} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{\ell_2})) \overline{D}_{e_2}v(x_{N^{**}-1}, x_{\ell_2}) \\ &\quad + \frac{\varepsilon^2}{4} \sum_{\ell_2=N^*+1}^{N^{**}-1} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{\ell_2-1})) \overline{D}_{e_2}v(x_{N^{**}-1}, x_{\ell_2}) \\ &\quad + \frac{\varepsilon^2}{4} \sum_{\ell_2=N^*}^{N^{**}-2} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{\ell_2})) \overline{D}_{e_2}v(x_{N^{**}+1}, x_{\ell_2}) \\ &\quad + \frac{\varepsilon^2}{4} \sum_{\ell_2=N^*+1}^{N^{**}-1} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{\ell_2-1})) \overline{D}_{e_2}v(x_{N^{**}+1}, x_{\ell_2}), \end{aligned} \quad (5.46)$$

the first variation of the interface energy  $\Gamma_3$  is:

$$\begin{aligned} \langle DE_{1,\Gamma_3}, v \rangle_{e_2} &= \frac{\varepsilon^2}{4} \sum_{\ell_1=N^*}^{N^{**}-2} \{ \nabla_\zeta \phi(\overline{D}_\eta y(x_{\ell_1}, x_{N^*-1})) \overline{D}_{e_2}v(x_{\ell_1}, x_{N^*-1}) \\ &\quad + \nabla_\zeta \phi(\overline{D}_\eta y(x_{\ell_1}, x_{N^*-1})) \overline{D}_{e_2}v(x_{\ell_1}, x_{N^*}) \} \\ &\quad + \frac{\varepsilon^2}{4} \sum_{\ell_1=N^*+2}^{N^{**}} \{ \nabla_\zeta \phi(\overline{D}_\eta y(x_{\ell_1-2}, x_{N^*-1})) \overline{D}_{e_2}v(x_{\ell_1}, x_{N^*-1}) \\ &\quad + \nabla_\zeta \phi(\overline{D}_\eta y(x_{\ell_1-2}, x_{N^*-1})) \overline{D}_{e_2}v(x_{\ell_1}, x_{N^*}) \}, \end{aligned} \quad (5.47)$$

and the first variation of the interface energy  $\Gamma_4$  is:

$$\begin{aligned}
\langle DE_{1,\Gamma_4}, v \rangle_{e_2} &= \frac{\varepsilon^2}{4} \sum_{\ell_2=N^*}^{N^{**}-2} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^*-1}, x_{\ell_2})) \overline{D}_{e_2} v(x_{N^*-1}, x_{\ell_2}) \\
&\quad + \frac{\varepsilon^2}{4} \sum_{\ell_2=N^*+1}^{N^{**}-1} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^*-1}, x_{\ell_2-1})) \overline{D}_{e_2} v(x_{N^*-1}, x_{\ell_2}) \\
&\quad + \frac{\varepsilon^2}{4} \sum_{\ell_2=N^*}^{N^{**}-2} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^*-1}, x_{\ell_2})) \overline{D}_{e_2} v(x_{N^*+1}, x_{\ell_2}) \\
&\quad + \frac{\varepsilon^2}{4} \sum_{\ell_2=N^*+1}^{N^{**}-1} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^*-1}, x_{\ell_2-1})) \overline{D}_{e_2} v(x_{N^*+1}, x_{\ell_2}).
\end{aligned} \tag{5.48}$$

For the corners, the first variation of the corner energy  $E_{C_1}$  is:

$$\begin{aligned}
\langle DE_{1,C_1}, v \rangle_{e_2} &= \frac{3\varepsilon^2}{8} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^*-1}, x_{N^{**}-1})) \{ \overline{D}_{e_2} v(x_{N^*-1}, x_{N^{**}-1}) \\
&\quad + \overline{D}_{e_2} v(x_{N^*-1}, x_{N^{**}}) \} + \frac{3\varepsilon^2}{8} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^*-1}, x_{N^{**}-1})) \\
&\quad \{ \overline{D}_{e_2} v(x_{N^*+1}, x_{N^{**}-1}) + \overline{D}_{e_2} v(x_{N^*+1}, x_{N^{**}}) \},
\end{aligned} \tag{5.49}$$

the first variation of the corner energy  $E_{C_2}$  is:

$$\begin{aligned}
\langle DE_{1,C_2}, v \rangle_{e_2} &= \frac{3\varepsilon^2}{8} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{N^{**}-1})) \{ \overline{D}_{e_2} v(x_{N^{**}-1}, x_{N^{**}-1}) \\
&\quad + \overline{D}_{e_2} v(x_{N^{**}-1}, x_{N^{**}}) \} + \frac{3\varepsilon^2}{8} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{N^{**}-1})) \\
&\quad \{ \overline{D}_{e_2} v(x_{N^{**}+1}, x_{N^{**}-1}) + \overline{D}_{e_2} v(x_{N^{**}+1}, x_{N^{**}}) \},
\end{aligned} \tag{5.50}$$

the first variation of the corner energy  $E_{C_3}$  is:

$$\begin{aligned}
\langle DE_{1,C_3}, v \rangle_{e_2} &= \frac{3\varepsilon^2}{8} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{N^*-1})) \{ \overline{D}_{e_2} v(x_{N^{**}-1}, x_{N^*-1}) \\
&\quad + \overline{D}_{e_2} v(x_{N^{**}-1}, x_{N^*}) \} + \frac{3\varepsilon^2}{8} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{N^*-1})) \\
&\quad \{ \overline{D}_{e_2} v(x_{N^{**}+1}, x_{N^*-1}) + \overline{D}_{e_2} v(x_{N^{**}+1}, x_{N^*}) \},
\end{aligned} \tag{5.51}$$

and finally, the first variation of the corner energy  $E_{C_4}$  is:

$$\begin{aligned}
\langle DE_{1,C_4}, v \rangle_{e_2} &= \frac{3\varepsilon^2}{8} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^*-1}, x_{N^*-1})) \{ \overline{D}_{e_2} v(x_{N^*-1}, x_{N^*-1}) \\
&\quad + \overline{D}_{e_2} v(x_{N^*-1}, x_{N^*}) \} + \frac{3\varepsilon^2}{8} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^*-1}, x_{N^*-1})) \\
&\quad \{ \overline{D}_{e_2} v(x_{N^*+1}, x_{N^*-1}) + \overline{D}_{e_2} v(x_{N^*+1}, x_{N^*}) \}.
\end{aligned} \tag{5.52}$$

### 5.2.2 Final reduction of the errors

Now, we will subtract the first variation of the bond volumes that intersect the interfaces as follows. First we will compute

$$W - \langle DE_{1,\Gamma_1}, v \rangle_{e_2} - \langle DE_{1,\Gamma_2}, v \rangle_{e_2} - \langle DE_{1,\Gamma_3}, v \rangle_{e_2} - \langle DE_{1,\Gamma_4}, v \rangle_{e_2}. \tag{5.53}$$

First, we will gather the terms along each interface. We will subtract the variation of the corners later on in our calculations (5.66)-(5.69) to prevent the equations being too long. Along interface  $\Gamma_1$  we have

$$\begin{aligned}
& \frac{\varepsilon^2}{2} \sum_{\ell_1=N^*-1}^{N^{**}-1} \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_{N^{**}-1})) + \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1-2}, x_{N^{**}-1})) \} \bar{D}_{e_2} v(x_{\ell_1}, x_{N^{**}}) \\
& - \frac{\varepsilon^2}{4} \sum_{\ell_1=N^*}^{N^{**}-2} \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_{N^{**}-1})) \bar{D}_{e_2} v(x_{\ell_1}, x_{N^{**}-1}) \\
& + \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_{N^{**}-1})) \} \bar{D}_{e_2} v(x_{\ell_1}, x_{N^{**}}) \} \\
& - \frac{\varepsilon^2}{4} \sum_{\ell_1=N^*+2}^{N^{**}} \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1-2}, x_{N^{**}-1})) \bar{D}_{e_2} v(x_{\ell_1}, x_{N^{**}-1}) \\
& + \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1-2}, x_{N^{**}-1})) \} \bar{D}_{e_2} v(x_{\ell_1}, x_{N^{**}}) \},
\end{aligned} \tag{5.54}$$

and along interface  $\Gamma_2$  we have

$$\begin{aligned}
& - \varepsilon^2 \sum_{\ell_2=N^*}^{N^{**}-1} \nabla_\zeta \phi(\nabla y(m_{(N^{**}-1, \ell_2)})) \bar{D}_{e_2} v(x_{N^{**}}, x_{\ell_2}) \\
& + \frac{\varepsilon^2}{2} \sum_{\ell_2=N^*-1}^{N^{**}-1} \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^{**}-2}, x_{\ell_2})) \bar{D}_{e_2} v(x_{N^{**}}, x_{\ell_2}) \\
& + \frac{\varepsilon^2}{2} \sum_{\ell_2=N^*}^{N^{**}} \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^{**}-2}, x_{\ell_2-1})) \bar{D}_{e_2} v(x_{N^{**}}, x_{\ell_2}) \\
& + \frac{\varepsilon^2}{2} \sum_{\ell_2=N^*-1}^{N^{**}-1} \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^{**}-1}, x_{\ell_2})) \bar{D}_{e_2} v(x_{N^{**}+1}, x_{\ell_2}) \\
& + \frac{\varepsilon^2}{2} \sum_{\ell_2=N^*}^{N^{**}} \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^{**}-1}, x_{\ell_2-1})) \bar{D}_{e_2} v(x_{N^{**}+1}, x_{\ell_2}) \\
& - \frac{\varepsilon^2}{4} \sum_{\ell_2=N^*}^{N^{**}-2} \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^{**}-1}, x_{\ell_2})) \bar{D}_{e_2} v(x_{N^{**}-1}, x_{\ell_2}) \\
& - \frac{\varepsilon^2}{4} \sum_{\ell_2=N^*+1}^{N^{**}-1} \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^{**}-1}, x_{\ell_2-1})) \bar{D}_{e_2} v(x_{N^{**}-1}, x_{\ell_2}) \\
& - \frac{\varepsilon^2}{4} \sum_{\ell_2=N^*}^{N^{**}-2} \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^{**}-1}, x_{\ell_2})) \bar{D}_{e_2} v(x_{N^{**}+1}, x_{\ell_2}) \\
& - \frac{\varepsilon^2}{4} \sum_{\ell_2=N^*+1}^{N^{**}-1} \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^{**}-1}, x_{\ell_2-1})) \bar{D}_{e_2} v(x_{N^{**}+1}, x_{\ell_2}).
\end{aligned} \tag{5.55}$$

Along interface  $\Gamma_3$  we have

$$\begin{aligned}
& \frac{\varepsilon^2}{2} \sum_{\ell_1=N^*-1}^{N^{**}-1} \{ \nabla_\zeta \phi(\overline{D}_\eta y(x_{\ell_1}, x_{N^*-1})) + \nabla_\zeta \phi(\overline{D}_\eta y(x_{\ell_1-2}, x_{N^*-1})) \} \overline{D}_{e_2} v(x_{\ell_1}, x_{N^*-1}) \\
& - \frac{\varepsilon^2}{4} \sum_{\ell_1=N^*}^{N^{**}-2} \{ \nabla_\zeta \phi(\overline{D}_\eta y(x_{\ell_1}, x_{N^*-1})) \overline{D}_{e_2} v(x_{\ell_1}, x_{N^*-1}) \\
& + \nabla_\zeta \phi(\overline{D}_\eta y(x_{\ell_1}, x_{N^*-1})) \} \overline{D}_{e_2} v(x_{\ell_1}, x_{N^*}) \} \\
& - \frac{\varepsilon^2}{4} \sum_{\ell_1=N^*+2}^{N^{**}} \{ \nabla_\zeta \phi(\overline{D}_\eta y(x_{\ell_1-2}, x_{N^*-1})) \overline{D}_{e_2} v(x_{\ell_1}, x_{N^*-1}) \\
& + \nabla_\zeta \phi(\overline{D}_\eta y(x_{\ell_1-2}, x_{N^*-1})) \overline{D}_{e_2} v(x_{\ell_1}, x_{N^*}) \}, \tag{5.56}
\end{aligned}$$

and along interface  $\Gamma_4$  we have

$$\begin{aligned}
& \varepsilon^2 \sum_{\ell_2=N^*}^{N^{**}-1} \nabla_\zeta \phi(\nabla y(m_{(N^*-1, \ell_2)})) \overline{D}_{e_2} v(x_{N^*}, x_{\ell_2}) \\
& - \frac{\varepsilon^2}{2} \sum_{\ell_2=N^*-1}^{N^{**}-1} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^*-2}, x_{\ell_2})) \overline{D}_{e_2} v(x_{N^*}, x_{\ell_2}) \\
& - \frac{\varepsilon^2}{2} \sum_{\ell_2=N^*}^{N^{**}} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^*-2}, x_{\ell_2-1})) \overline{D}_{e_2} v(x_{N^*}, x_{\ell_2}) \\
& + \frac{\varepsilon^2}{2} \sum_{\ell_2=N^*}^{N^{**}-1} \{ \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^*-1}, x_{\ell_2})) + \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^*-1}, x_{\ell_2-1})) \} \overline{D}_{e_2} v(x_{N^*-1}, x_{\ell_2}) \\
& - \frac{\varepsilon^2}{2} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^*-3}, x_{N^*-1})) \overline{D}_{e_2} v(x_{N^*-1}, x_{N^*-1}) \\
& - \frac{\varepsilon^2}{2} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^*-3}, x_{N^{**}-1})) \overline{D}_{e_2} v(x_{N^*-1}, x_{N^{**}}) \\
& - \frac{\varepsilon^2}{4} \sum_{\ell_2=N^*}^{N^{**}-2} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^*-1}, x_{\ell_2})) \overline{D}_{e_2} v(x_{N^*-1}, x_{\ell_2}) \\
& - \frac{\varepsilon^2}{4} \sum_{\ell_2=N^*+1}^{N^{**}-1} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^*-1}, x_{\ell_2-1})) \overline{D}_{e_2} v(x_{N^*-1}, x_{\ell_2}) \\
& - \frac{\varepsilon^2}{4} \sum_{\ell_2=N^*}^{N^{**}-2} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^*-1}, x_{\ell_2})) \overline{D}_{e_2} v(x_{N^*+1}, x_{\ell_2}) \\
& - \frac{\varepsilon^2}{4} \sum_{\ell_2=N^*+1}^{N^{**}-1} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^*-1}, x_{\ell_2-1})) \overline{D}_{e_2} v(x_{N^*+1}, x_{\ell_2}). \tag{5.57}
\end{aligned}$$

We will rewrite all the terms in terms of the original indexing ( $\ell_1, \ell_2 = N^*, \dots, N^{**}-1$ ) for convenience.

After re-indexing (5.54), we have along interface  $\Gamma_1$  the following terms

$$\begin{aligned}
& \frac{\varepsilon^2}{2} \sum_{\ell_1=N^*}^{N^{**}-1} \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_{N^{**}-1})) + \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1-2}, x_{N^{**}-1})) \} \bar{D}_{e_2} v(x_{\ell_1}, x_{N^{**}}) \\
& + \frac{\varepsilon^2}{2} \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^*-1}, x_{N^{**}-1})) + \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^*-3}, x_{N^{**}-1})) \} \bar{D}_{e_2} v(x_{N^*-1}, x_{N^{**}}) \\
& - \frac{\varepsilon^2}{4} \sum_{\ell_1=N^*}^{N^{**}-1} \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_{N^{**}-1})) \} \bar{D}_{e_2} v(x_{\ell_1}, x_{N^{**}-1}) \\
& + \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_{N^{**}-1})) \bar{D}_{e_2} v(x_{\ell_1}, x_{N^{**}}) \} \\
& + \frac{\varepsilon^2}{4} \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^{**}-1}, x_{N^{**}-1})) \} \bar{D}_{e_2} v(x_{N^{**}-1}, x_{N^{**}-1}) \\
& + \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^{**}-1}, x_{N^{**}-1})) \bar{D}_{e_2} v(x_{N^{**}-1}, x_{N^{**}}) \} \\
& - \frac{\varepsilon^2}{4} \sum_{\ell_1=N^*}^{N^{**}-1} \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1-2}, x_{N^{**}-1})) \} \bar{D}_{e_2} v(x_{\ell_1}, x_{N^{**}-1}) \\
& + \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1-2}, x_{N^{**}-1})) \bar{D}_{e_2} v(x_{\ell_1}, x_{N^{**}}) \} \\
& - \frac{\varepsilon^2}{4} \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^{**}-2}, x_{N^{**}-1})) \} \bar{D}_{e_2} v(x_{N^{**}}, x_{N^{**}-1}) \\
& + \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^{**}-2}, x_{N^{**}-1})) \bar{D}_{e_2} v(x_{N^{**}}, x_{N^{**}}) \} \\
& + \frac{\varepsilon^2}{4} \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^*-2}, x_{N^{**}-1})) \} \bar{D}_{e_2} v(x_{N^*}, x_{N^{**}-1}) \\
& + \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^*-2}, x_{N^{**}-1})) \bar{D}_{e_2} v(x_{N^*}, x_{N^{**}}) \} \\
& + \frac{\varepsilon^2}{4} \{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^*-1}, x_{N^{**}-1})) \} \bar{D}_{e_2} v(x_{N^*+1}, x_{N^{**}-1}) \\
& + \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^*-1}, x_{N^{**}-1})) \bar{D}_{e_2} v(x_{N^*+1}, x_{N^{**}}) \}.
\end{aligned} \tag{5.58}$$

After re-indexing (5.55) along interface  $\Gamma_2$  we have

$$\begin{aligned}
& \varepsilon^2 \sum_{\ell_2=N^*}^{N^{**}-1} \left\{ -\nabla_\zeta \phi(\nabla y(m_{(N^{**}-1, \ell_2)})) + \frac{1}{2} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-2}, x_{\ell_2})) \right. \\
& + \frac{1}{2} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-2}, x_{\ell_2-1}))) \} \overline{D}_{e_2} v(x_{N^{**}}, x_{\ell_2}) \\
& + \frac{\varepsilon^2}{2} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-2}, x_{N^*-1})) \overline{D}_{e_2} v(x_{N^{**}}, x_{N^*-1}) \\
& + \frac{\varepsilon^2}{2} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-2}, x_{N^{**}-1})) \overline{D}_{e_2} v(x_{N^{**}}, x_{N^{**}}) \\
& + \frac{\varepsilon^2}{2} \sum_{\ell_2=N^*}^{N^{**}-1} \left\{ \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{\ell_2})) + \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{\ell_2-1})) \right\} \overline{D}_{e_2} v(x_{N^{**}+1}, x_{\ell_2}) \\
& + \frac{\varepsilon^2}{2} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{N^*-1})) \overline{D}_{e_2} v(x_{N^{**}+1}, x_{N^*-1}) \\
& + \frac{\varepsilon^2}{2} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{N^{**}-1})) \overline{D}_{e_2} v(x_{N^{**}+1}, x_{N^{**}}) \\
& - \frac{\varepsilon^2}{4} \sum_{\ell_2=N^*}^{N^{**}-1} \left\{ \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{\ell_2})) + \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{\ell_2-1})) \right\} \overline{D}_{e_2} v(x_{N^{**}-1}, x_{\ell_2}) \\
& - \frac{\varepsilon^2}{4} \sum_{\ell_2=N^*}^{N^{**}-1} \left\{ \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{\ell_2})) + \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{\ell_2-1})) \right\} \overline{D}_{e_2} v(x_{N^{**}+1}, x_{\ell_2}) \\
& + \frac{\varepsilon^2}{4} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{N^{**}-1})) \overline{D}_{e_2} v(x_{N^{**}-1}, x_{N^{**}-1}) \\
& + \frac{\varepsilon^2}{4} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{N^*-1})) \overline{D}_{e_2} v(x_{N^{**}-1}, x_{N^*}) \\
& + \frac{\varepsilon^2}{4} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{N^{**}-1})) \overline{D}_{e_2} v(x_{N^{**}+1}, x_{N^{**}-1}) \\
& + \frac{\varepsilon^2}{4} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{N^*-1})) \overline{D}_{e_2} v(x_{N^{**}+1}, x_{N^*}).
\end{aligned} \tag{5.59}$$



By re-indexing (5.56) we have along interface  $\Gamma_3$

$$\begin{aligned}
& \frac{\varepsilon^2}{2} \sum_{\ell_1=N^*}^{N^{**}-1} \{ \nabla_\zeta \phi(\overline{D}_\eta y(x_{\ell_1}, x_{N^*-1})) + \nabla_\zeta \phi(\overline{D}_\eta y(x_{\ell_1-2}, x_{N^*-1})) \} \overline{D}_{e_2} v(x_{\ell_1}, x_{N^*-1}) \\
& + \frac{\varepsilon^2}{2} \{ \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^*-1}, x_{N^*-1})) + \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^*-3}, x_{N^*-1})) \} \overline{D}_{e_2} v(x_{N^*-1}, x_{N^*-1}) \\
& - \frac{\varepsilon^2}{4} \sum_{\ell_1=N^*}^{N^{**}-1} \{ \nabla_\zeta \phi(\overline{D}_\eta y(x_{\ell_1}, x_{N^*-1})) \overline{D}_{e_2} v(x_{\ell_1}, x_{N^*-1}) \\
& + \nabla_\zeta \phi(\overline{D}_\eta y(x_{\ell_1}, x_{N^*-1})) \overline{D}_{e_2} v(x_{\ell_1}, x_{N^*}) \} \\
& - \frac{\varepsilon^2}{4} \sum_{\ell_1=N^*}^{N^{**}-1} \{ \nabla_\zeta \phi(\overline{D}_\eta y(x_{\ell_1-2}, x_{N^*-1})) \overline{D}_{e_2} v(x_{\ell_1}, x_{N^*-1}) \\
& + \nabla_\zeta \phi(\overline{D}_\eta y(x_{\ell_1-2}, x_{N^*-1})) \overline{D}_{e_2} v(x_{\ell_1}, x_{N^*}) \} \\
& + \frac{\varepsilon^2}{4} \{ \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{N^*-1})) \overline{D}_{e_2} v(x_{N^{**}-1}, x_{N^*-1}) \\
& + \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{N^*-1})) \overline{D}_{e_2} v(x_{N^{**}-1}, x_{N^*}) \} \\
& + \frac{\varepsilon^2}{4} \{ \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^*-2}, x_{N^*-1})) \overline{D}_{e_2} v(x_{N^*}, x_{N^*-1}) \\
& + \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^*-2}, x_{N^*-1})) \overline{D}_{e_2} v(x_{N^*}, x_{N^*}) \} \\
& + \frac{\varepsilon^2}{4} \{ \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^*-1}, x_{N^*-1})) \overline{D}_{e_2} v(x_{N^*+1}, x_{N^*-1}) \\
& + \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^*-1}, x_{N^*-1})) \overline{D}_{e_2} v(x_{N^*+1}, x_{N^*}) \} \\
& - \frac{\varepsilon^2}{4} \{ \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-2}, x_{N^*-1})) \overline{D}_{e_2} v(x_{N^{**}}, x_{N^*-1}) \\
& + \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-2}, x_{N^*-1})) \overline{D}_{e_2} v(x_{N^*+1}, x_{N^*}) \},
\end{aligned} \tag{5.60}$$

and finally, by re-indexing (5.57) we have along interface  $\Gamma_4$

$$\begin{aligned}
& \varepsilon^2 \sum_{\ell_2=N^*}^{N^{**}-1} \left\{ \nabla_\zeta \phi(\nabla y(m_{(N^*-1, \ell_2)})) - \frac{1}{2} \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^*-2}, x_{\ell_2})) \right. \\
& \quad - \frac{1}{2} \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^*-2}, x_{\ell_2-1})) \left. \right\} \bar{D}_{e_2} v(x_{N^*}, x_{\ell_2}) \\
& \quad - \frac{\varepsilon^2}{2} \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^*-2}, x_{N^*-1})) \bar{D}_{e_2} v(x_{N^*}, x_{N^*-1}) \\
& \quad - \frac{\varepsilon^2}{2} \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^*-2}, x_{N^{**}-1})) \bar{D}_{e_2} v(x_{N^*}, x_{N^{**}}) \\
& \quad + \frac{\varepsilon^2}{2} \sum_{\ell_2=N^*}^{N^{**}-1} \left\{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^*-1}, x_{\ell_2})) \right. \\
& \quad + \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^*-1}, x_{\ell_2-1})) \left. \right\} \bar{D}_{e_2} v(x_{N^*-1}, x_{\ell_2}) \\
& \quad - \frac{\varepsilon^2}{2} \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^*-3}, x_{N^*-1})) \bar{D}_{e_2} v(x_{N^*-1}, x_{N^*-1}) \\
& \quad - \frac{\varepsilon^2}{2} \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^*-3}, x_{N^{**}-1})) \bar{D}_{e_2} v(x_{N^*-1}, x_{N^{**}}) \\
& \quad - \frac{\varepsilon^2}{4} \sum_{\ell_2=N^*}^{N^{**}-1} \left\{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^*-1}, x_{\ell_2})) + \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^*-1}, x_{\ell_2-1})) \right\} \bar{D}_{e_2} v(x_{N^*-1}, x_{\ell_2}) \\
& \quad - \frac{\varepsilon^2}{4} \sum_{\ell_2=N^*}^{N^{**}-1} \left\{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^*-1}, x_{\ell_2})) + \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^*-1}, x_{\ell_2-1})) \right\} \bar{D}_{e_2} v(x_{N^*+1}, x_{\ell_2}) \\
& \quad + \frac{\varepsilon^2}{4} \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^*-1}, x_{N^{**}-1})) \bar{D}_{e_2} v(x_{N^*-1}, x_{N^{**}-1}) \\
& \quad + \frac{\varepsilon^2}{4} \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^*-1}, x_{N^*-1})) \bar{D}_{e_2} v(x_{N^*-1}, x_{N^*}) \\
& \quad + \frac{\varepsilon^2}{4} \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^*-1}, x_{N^{**}-1})) \bar{D}_{e_2} v(x_{N^*+1}, x_{N^{**}-1}) \\
& \quad + \frac{\varepsilon^2}{4} \nabla_\zeta \phi(\bar{D}_\eta y(x_{N^*-1}, x_{N^*-1})) \bar{D}_{e_2} v(x_{N^*+1}, x_{N^*}).
\end{aligned} \tag{5.61}$$

Now we will keep the summation terms on each interface (5.58)-(5.61) and then the rest of the terms will be grouped along the corners of the interfaces. This step makes it easier to see what needs to be added to the energy on the interface, specifically what the  $E_2$  terms will be.

Along interface  $\Gamma_1$  we have

$$\begin{aligned}
& \frac{\varepsilon^2}{2} \sum_{\ell_1=N^*}^{N^{**}-1} \left\{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_{N^{**}-1})) + \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1-2}, x_{N^{**}-1})) \right\} \bar{D}_{e_2} v(x_{\ell_1}, x_{N^{**}}) \\
& \quad - \frac{\varepsilon^2}{4} \sum_{\ell_1=N^*}^{N^{**}-1} \left\{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_{N^{**}-1})) + \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1-2}, x_{N^{**}-1})) \right\} \bar{D}_{e_2} v(x_{\ell_1}, x_{N^{**}-1}) \\
& \quad - \frac{\varepsilon^2}{4} \sum_{\ell_1=N^*}^{N^{**}-1} \left\{ \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_{N^{**}-1})) + \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1-2}, x_{N^{**}-1})) \right\} \bar{D}_{e_2} v(x_{\ell_1}, x_{N^{**}}),
\end{aligned} \tag{5.62}$$

along interface  $\Gamma_2$  we have

$$\begin{aligned}
& \varepsilon^2 \sum_{\ell_2=N^*}^{N^{**}-1} \left\{ -\nabla_\zeta \phi(\nabla y(m_{(N^{**}-1, \ell_2)})) + \frac{1}{2} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-2}, x_{\ell_2})) \right. \\
& + \frac{1}{2} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-2}, x_{\ell_2-1}))) \} \overline{D}_{e_2} v(x_{N^{**}}, x_{\ell_2}) \\
& + \frac{\varepsilon^2}{2} \sum_{\ell_2=N^*}^{N^{**}-1} \left\{ \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{\ell_2})) + \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{\ell_2-1})) \right\} \overline{D}_{e_2} v(x_{N^{**}+1}, x_{\ell_2}) \\
& - \frac{\varepsilon^2}{4} \sum_{\ell_2=N^*}^{N^{**}-1} \left\{ \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{\ell_2})) + \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{\ell_2-1})) \right\} \overline{D}_{e_2} v(x_{N^{**}-1}, x_{\ell_2}) \\
& - \frac{\varepsilon^2}{4} \sum_{\ell_2=N^*}^{N^{**}-1} \left\{ \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{\ell_2})) + \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{\ell_2-1})) \right\} \overline{D}_{e_2} v(x_{N^{**}+1}, x_{\ell_2}).
\end{aligned} \tag{5.63}$$

Along interface  $\Gamma_3$  we have

$$\begin{aligned}
& \frac{\varepsilon^2}{2} \sum_{\ell_1=N^*}^{N^{**}-1} \left\{ \nabla_\zeta \phi(\overline{D}_\eta y(x_{\ell_1}, x_{N^*-1})) + \nabla_\zeta \phi(\overline{D}_\eta y(x_{\ell_1-2}, x_{N^*-1})) \right\} \overline{D}_{e_2} v(x_{\ell_1}, x_{N^*-1}) \\
& - \frac{\varepsilon^2}{4} \sum_{\ell_1=N^*}^{N^{**}-1} \left\{ \nabla_\zeta \phi(\overline{D}_\eta y(x_{\ell_1}, x_{N^*-1})) + \nabla_\zeta \phi(\overline{D}_\eta y(x_{\ell_1-2}, x_{N^*-1})) \right\} \overline{D}_{e_2} v(x_{\ell_1}, x_{N^*-1}) \\
& - \frac{\varepsilon^2}{4} \sum_{\ell_1=N^*}^{N^{**}-1} \left\{ \nabla_\zeta \phi(\overline{D}_\eta y(x_{\ell_1}, x_{N^*-1})) + \nabla_\zeta \phi(\overline{D}_\eta y(x_{\ell_1-2}, x_{N^*-1})) \right\} \overline{D}_{e_2} v(x_{\ell_1}, x_{N^*}),
\end{aligned} \tag{5.64}$$

and finally, along interface  $\Gamma_4$  we have

$$\begin{aligned}
& \varepsilon^2 \sum_{\ell_2=N^*}^{N^{**}-1} \left\{ \nabla_\zeta \phi(\nabla y(m_{(N^*-1, \ell_2)})) - \frac{1}{2} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^*-2}, x_{\ell_2})) \right. \\
& - \frac{1}{2} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^*-2}, x_{\ell_2-1}))) \} \overline{D}_{e_2} v(x_{N^*}, x_{\ell_2}) \\
& + \frac{\varepsilon^2}{2} \sum_{\ell_2=N^*}^{N^{**}-1} \left\{ \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^*-1}, x_{\ell_2})) + \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^*-1}, x_{\ell_2-1})) \right\} \overline{D}_{e_2} v(x_{N^*-1}, x_{\ell_2}) \\
& - \frac{\varepsilon^2}{4} \sum_{\ell_2=N^*}^{N^{**}-1} \left\{ \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^*-1}, x_{\ell_2})) + \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^*-1}, x_{\ell_2-1})) \right\} \overline{D}_{e_2} v(x_{N^*-1}, x_{\ell_2}) \\
& - \frac{\varepsilon^2}{4} \sum_{\ell_2=N^*}^{N^{**}-1} \left\{ \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^*-1}, x_{\ell_2})) + \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^*-1}, x_{\ell_2-1})) \right\} \overline{D}_{e_2} v(x_{N^*+1}, x_{\ell_2}).
\end{aligned} \tag{5.65}$$

When grouping the rest of the terms we also subtract the first variation of the corners, namely  $\langle DE_{C_1}, v \rangle_{e_2}, \langle DE_{C_2}, v \rangle_{e_2}, \langle DE_{C_3}, v \rangle_{e_2}$  and  $\langle DE_{C_4}, v \rangle_{e_2}$ , (5.49)-(5.52).

Along corner  $C_1$  we have

$$\begin{aligned}
& \frac{\varepsilon^2}{2} \{ \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^*-1}, x_{N^{**}-1})) + \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^*-3}, x_{N^{**}-1})) \} \overline{D}_{e_2} v(x_{N^*-1}, x_{N^{**}}) \\
& + \frac{\varepsilon^2}{4} \{ \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^*-2}, x_{N^{**}-1})) \overline{D}_{e_2} v(x_{N^*}, x_{N^{**}-1}) \\
& + \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^*-2}, x_{N^{**}-1})) \} \overline{D}_{e_2} v(x_{N^*}, x_{N^{**}}) \} \\
& + \frac{\varepsilon^2}{4} \{ \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^*-1}, x_{N^{**}-1})) \overline{D}_{e_2} v(x_{N^*+1}, x_{N^{**}-1}) \\
& + \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^*-1}, x_{N^{**}-1})) \} \overline{D}_{e_2} v(x_{N^*+1}, x_{N^{**}}) \} \\
& - \frac{\varepsilon^2}{2} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^*-2}, x_{N^{**}-1})) \overline{D}_{e_2} v(x_{N^*}, x_{N^{**}}) \\
& - \frac{\varepsilon^2}{2} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^*-3}, x_{N^{**}-1})) \overline{D}_{e_2} v(x_{N^*-1}, x_{N^{**}}) \} \\
& + \frac{\varepsilon^2}{4} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^*-1}, x_{N^{**}-1})) \overline{D}_{e_2} v(x_{N^*-1}, x_{N^{**}-1}) \\
& + \frac{\varepsilon^2}{4} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^*-1}, x_{N^{**}-1})) \overline{D}_{e_2} v(x_{N^*+1}, x_{N^{**}-1}) \} \\
& - \frac{3\varepsilon^2}{8} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^*-1}, x_{N^{**}-1})) \{ \overline{D}_{e_2} v(x_{N^*-1}, x_{N^{**}-1}) + \overline{D}_{e_2} v(x_{N^*-1}, x_{N^{**}}) \} \\
& - \frac{3\varepsilon^2}{8} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^*-1}, x_{N^{**}-1})) \{ \overline{D}_{e_2} v(x_{N^*+1}, x_{N^{**}-1}) + \overline{D}_{e_2} v(x_{N^*+1}, x_{N^{**}}) \},
\end{aligned} \tag{5.66}$$

along corner  $C_2$  we have

$$\begin{aligned}
& \frac{\varepsilon^2}{4} \{ \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{N^{**}-1})) \overline{D}_{e_2} v(x_{N^{**}-1}, x_{N^{**}-1}) \\
& + \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{N^{**}-1})) \overline{D}_{e_2} v(x_{N^{**}-1}, x_{N^{**}}) \} \\
& - \frac{\varepsilon^2}{4} \{ \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-2}, x_{N^{**}-1})) \overline{D}_{e_2} v(x_{N^{**}}, x_{N^{**}-1}) \\
& + \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-2}, x_{N^{**}-1})) \overline{D}_{e_2} v(x_{N^{**}}, x_{N^{**}}) \} \\
& + \frac{\varepsilon^2}{2} \{ \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-2}, x_{N^{**}-1})) \overline{D}_{e_2} v(x_{N^{**}}, x_{N^{**}}) \\
& + \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{N^{**}-1})) \overline{D}_{e_2} v(x_{N^{**}+1}, x_{N^{**}}) \} \\
& + \frac{\varepsilon^2}{4} \{ \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{N^{**}-1})) \overline{D}_{e_2} v(x_{N^{**}-1}, x_{N^{**}-1}) \\
& + \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{N^{**}-1})) \overline{D}_{e_2} v(x_{N^{**}+1}, x_{N^{**}-1}) \\
& - \frac{3\varepsilon^2}{8} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{N^{**}-1})) \{ \overline{D}_{e_2} v(x_{N^{**}-1}, x_{N^{**}-1}) + \overline{D}_{e_2} v(x_{N^{**}-1}, x_{N^{**}}) \} \\
& - \frac{3\varepsilon^2}{8} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{N^{**}-1})) \{ \overline{D}_{e_2} v(x_{N^{**}+1}, x_{N^{**}-1}) + \overline{D}_{e_2} v(x_{N^{**}+1}, x_{N^{**}}) \}.
\end{aligned} \tag{5.67}$$

Along corner  $C_3$  we have

$$\begin{aligned}
& \frac{\varepsilon^2}{2} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-2}, x_{N^*-1})) \overline{D}_{e_2} v(x_{N^{**}}, x_{N^*-1}) \\
& + \frac{\varepsilon^2}{2} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{N^*-1})) \overline{D}_{e_2} v(x_{N^{**}+1}, x_{N^*-1}) \\
& + \frac{\varepsilon^2}{4} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{N^*-1})) \overline{D}_{e_2} v(x_{N^{**}-1}, x_{N^*}) \\
& + \frac{\varepsilon^2}{4} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{N^*-1})) \overline{D}_{e_2} v(x_{N^{**}+1}, x_{N^*}) \\
& + \frac{\varepsilon^2}{4} \{ \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{N^*-1})) \overline{D}_{e_2} v(x_{N^{**}-1}, x_{N^*-1}) \\
& + \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{N^*-1})) \overline{D}_{e_2} v(x_{N^{**}-1}, x_{N^*}) \} \\
& - \frac{\varepsilon^2}{4} \{ \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-2}, x_{N^*-1})) \overline{D}_{e_2} v(x_{N^{**}}, x_{N^*-1}) \\
& + \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-2}, x_{N^*-1})) \overline{D}_{e_2} v(x_{N^{**}}, x_{N^*}) \} \\
& - \frac{3\varepsilon^2}{8} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{N^*-1})) \{ \overline{D}_{e_2} v(x_{N^{**}-1}, x_{N^*-1}) + \overline{D}_{e_2} v(x_{N^{**}-1}, x_{N^*}) \} \\
& - \frac{3\varepsilon^2}{8} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{N^*-1})) \{ \overline{D}_{e_2} v(x_{N^{**}+1}, x_{N^*-1}) + \overline{D}_{e_2} v(x_{N^{**}+1}, x_{N^*}) \},
\end{aligned} \tag{5.68}$$

and finally along corner  $C_4$  we have

$$\begin{aligned}
& \frac{\varepsilon^2}{2} \{ \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^*-1}, x_{N^*-1})) + \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^*-3}, x_{N^*-1})) \} \overline{D}_{e_2} v(x_{N^*-1}, x_{N^*-1}) \\
& + \frac{\varepsilon^2}{4} \{ \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^*-2}, x_{N^*-1})) \overline{D}_{e_2} v(x_{N^*}, x_{N^*-1}) \\
& + \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^*-2}, x_{N^*-1})) \overline{D}_{e_2} v(x_{N^*}, x_{N^*}) \} \\
& + \frac{\varepsilon^2}{4} \{ \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^*-1}, x_{N^*-1})) \overline{D}_{e_2} v(x_{N^*+1}, x_{N^*-1}) \\
& + \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^*-1}, x_{N^*-1})) \overline{D}_{e_2} v(x_{N^*+1}, x_{N^*}) \} \\
& - \frac{\varepsilon^2}{2} \{ \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^*-2}, x_{N^*-1})) \overline{D}_{e_2} v(x_{N^*}, x_{N^*-1}) \\
& + \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^*-3}, x_{N^*-1})) \overline{D}_{e_2} v(x_{N^*-1}, x_{N^*-1}) \} \\
& + \frac{\varepsilon^2}{4} \{ \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^*-1}, x_{N^*-1})) \overline{D}_{e_2} v(x_{N^*-1}, x_{N^*}) \\
& + \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^*-1}, x_{N^*-1})) \overline{D}_{e_2} v(x_{N^*+1}, x_{N^*}) \} \\
& - \frac{3\varepsilon^2}{8} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^*-1}, x_{N^*-1})) \{ \overline{D}_{e_2} v(x_{N^*-1}, x_{N^*-1}) + \overline{D}_{e_2} v(x_{N^*-1}, x_{N^*}) \} \\
& - \frac{3\varepsilon^2}{8} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^*-1}, x_{N^*-1})) \{ \overline{D}_{e_2} v(x_{N^*+1}, x_{N^*-1}) + \overline{D}_{e_2} v(x_{N^*+1}, x_{N^*}) \}.
\end{aligned} \tag{5.69}$$

Recall that the aim of the calculations for the first variation of the difference between the atomistic Cauchy-Born energy and the coupled energy is to achieve a satisfactory error. In order to do this we have to cancel out the terms (5.62)-(5.69). This is done

by subtracting from the energy on the interface  $E_{\Gamma,\eta}$  some terms, the  $E_2$  terms, whose first variation cancel out with the terms in (5.62)-(5.69). This is why the energy on the interfaces and the corners has the form as in Section 4.6. Now we will compute the first variation of the energy on the interfaces and the corners without including their first term whose first variation has been computed earlier on in this chapter.

### 5.2.3 First Variation of $E_2$ interface terms

Now we focus on the second term,  $E_2$ , of the energy on the interface, (5.32). Recall in Section 4.6, the energy on each interface. For interface  $\Gamma_1$ , the  $E_2$  term is

$$\begin{aligned}
E_{2,\Gamma_1}\{y\} = & -\frac{\varepsilon^2}{4} \sum_{\ell_1=N^*}^{N^{**}-1} \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_{N^{**}-1})) [\bar{D}_{e_2} y(x_{\ell_1}, x_{N^{**}-1}) - \bar{D}_{e_2} y(x_{\ell_1}, x_{N^{**}})] \\
& -\frac{\varepsilon^2}{4} \sum_{\ell_1=N^*}^{N^{**}-1} \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1-2}, x_{N^{**}-1})) [\bar{D}_{e_2} y(x_{\ell_1}, x_{N^{**}-1}) - \bar{D}_{e_2} y(x_{\ell_1}, x_{N^{**}})] \\
& -\frac{\varepsilon^2}{4} \sum_{\ell_1=N^*}^{N^{**}-1} \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_{N^{**}-1})) [\bar{D}_{e_1} y(x_{\ell_1}, x_{N^{**}+1}) - \bar{D}_{e_1} y(x_{\ell_1}, x_{N^{**}-1})] \\
& -\frac{\varepsilon^2}{4} \sum_{\ell_1=N^*}^{N^{**}-1} \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1-1}, x_{N^{**}-1})) [\bar{D}_{e_1} y(x_{\ell_1}, x_{N^{**}+1}) \\
& - \bar{D}_{e_1} y(x_{\ell_1}, x_{N^{**}-1})].
\end{aligned} \tag{5.70}$$

Again, we will focus only on the  $\bar{D}_{e_2}$  terms and  $\langle \cdot, \cdot \rangle_{e_2}$  will denote the terms in the  $e_2$  direction of  $\langle \cdot, \cdot \rangle_\varepsilon$ . The calculations for the first variation are in Appendix A. The first variation of  $E_{2,\Gamma_1}$  in the  $e_2$  direction is

$$\begin{aligned}
\langle DE_{2,\Gamma_1}\{y\}, v \rangle_{e_2} = & -\frac{\varepsilon^2}{4} \sum_{\ell_1=N^*}^{N^{**}-1} \nabla_\zeta^2 \phi(\bar{D}_\eta y(x_{\ell_1}, x_{N^{**}-1})) \{ \bar{D}_{e_2} y(x_{\ell_1}, x_{N^{**}-1}) \\
& - \bar{D}_{e_2} y(x_{\ell_1}, x_{N^{**}}) \} \bar{D}_\eta v(x_{\ell_1}, x_{N^{**}-1}) \\
& -\frac{\varepsilon^2}{4} \sum_{\ell_1=N^*}^{N^{**}-1} \nabla_\zeta^2 \phi(\bar{D}_\eta y(x_{\ell_1-2}, x_{N^{**}-1})) \{ \bar{D}_{e_2} y(x_{\ell_1}, x_{N^{**}-1}) \\
& - \bar{D}_{e_2} y(x_{\ell_1}, x_{N^{**}}) \} \bar{D}_\eta v(x_{\ell_1-2}, x_{N^{**}-1}) \\
& -\frac{\varepsilon^2}{4} \sum_{\ell_1=N^*}^{N^{**}-1} \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1}, x_{N^{**}-1})) \{ \bar{D}_{e_2} v(x_{\ell_1}, x_{N^{**}-1}) \\
& - \bar{D}_{e_2} v(x_{\ell_1}, x_{N^{**}}) \} - \frac{\varepsilon^2}{4} \sum_{\ell_1=N^*}^{N^{**}-1} \nabla_\zeta \phi(\bar{D}_\eta y(x_{\ell_1-2}, x_{N^{**}-1})) \\
& \{ \bar{D}_{e_2} v(x_{\ell_1}, x_{N^{**}-1}) - \bar{D}_{e_2} v(x_{\ell_1}, x_{N^{**}}) \}.
\end{aligned} \tag{5.71}$$

The first variation of  $E_{2,\Gamma_2}$  in the  $e_2$  direction is

$$\begin{aligned}
\langle DE_{2,\Gamma_2}\{y\}, v \rangle_{e_2} = & -\frac{\varepsilon^2}{4} \sum_{\ell_2=N^*}^{N^{**}-1} \nabla_\zeta^2 \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{\ell_2})) \{ \overline{D}_{e_2} y(x_{N^{**}-1}, x_{\ell_2}) \\
& - \overline{D}_{e_2} y(x_{N^{**}+1}, x_{\ell_2}) \} \overline{D}_\eta v(x_{N^{**}-1}, x_{\ell_2}) \\
& - \frac{\varepsilon^2}{4} \sum_{\ell_2=N^*}^{N^{**}-1} \nabla_\zeta^2 \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{\ell_2-1})) \{ \overline{D}_{e_2} y(x_{N^{**}-1}, x_{\ell_2}) \\
& - \overline{D}_{e_2} y(x_{N^{**}+1}, x_{\ell_2}) \} \overline{D}_\eta v(x_{N^{**}-1}, x_{\ell_2-1}) \\
& - \frac{\varepsilon^2}{4} \sum_{\ell_2=N^*}^{N^{**}-1} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{\ell_2})) \{ \overline{D}_{e_2} v(x_{N^{**}-1}, x_{\ell_2}) \\
& - \overline{D}_{e_2} v(x_{N^{**}+1}, x_{\ell_2}) \} - \frac{\varepsilon^2}{4} \sum_{\ell_2=N^*}^{N^{**}-1} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{\ell_2-1})) \\
& \{ \overline{D}_{e_2} v(x_{N^{**}-1}, x_{\ell_2}) - \overline{D}_{e_2} v(x_{N^{**}+1}, x_{\ell_2}) \}.
\end{aligned} \tag{5.72}$$

The first variation of  $E_{2,\Gamma_3}$  in the  $e_2$  direction is

$$\begin{aligned}
\langle DE_{2,\Gamma_3}\{y\}, v \rangle_{e_2} = & -\frac{\varepsilon^2}{4} \sum_{\ell_1=N^*}^{N^{**}-1} \nabla_\zeta^2 \phi(\overline{D}_\eta y(x_{\ell_1}, x_{N^*-1})) \{ \overline{D}_{e_2} y(x_{\ell_1}, x_{N^*}) \\
& - \overline{D}_{e_2} y(x_{\ell_1}, x_{N^*-1}) \} \overline{D}_\eta v(x_{\ell_1}, x_{N^*-1}) \\
& - \frac{\varepsilon^2}{4} \sum_{\ell_1=N^*}^{N^{**}-1} \nabla_\zeta^2 \phi(\overline{D}_\eta y(x_{\ell_1-2}, x_{N^*-1})) \{ \overline{D}_{e_2} y(x_{\ell_1}, x_{N^*}) \\
& - \overline{D}_{e_2} y(x_{\ell_1}, x_{N^*-1}) \} \overline{D}_\eta v(x_{\ell_1-2}, x_{N^*-1}) \\
& - \frac{\varepsilon^2}{4} \sum_{\ell_1=N^*}^{N^{**}-1} \nabla_\zeta \phi(\overline{D}_\eta y(x_{\ell_1}, x_{N^*-1})) \{ \overline{D}_{e_2} v(x_{\ell_1}, x_{N^*}) \\
& - \overline{D}_{e_2} v(x_{\ell_1}, x_{N^*-1}) \} - \frac{\varepsilon^2}{4} \sum_{\ell_1=N^*}^{N^{**}-1} \nabla_\zeta \phi(\overline{D}_\eta y(x_{\ell_1-2}, x_{N^*-1})) \\
& \{ \overline{D}_{e_2} v(x_{\ell_1}, x_{N^*}) - \overline{D}_{e_2} v(x_{\ell_1}, x_{N^*-1}) \}.
\end{aligned} \tag{5.73}$$

The first variation of  $E_{2,\Gamma_4}$  in the  $e_2$  direction is

$$\begin{aligned}
\langle DE_{2,\Gamma_4}\{y\}, v \rangle_{e_2} = & -\frac{\varepsilon^2}{4} \sum_{\ell_2=N^*}^{N^{**}-1} \nabla_\zeta^2 \phi(\overline{D}_\eta y(x_{N^*-1}, x_{\ell_2})) \{ \overline{D}_{e_2} y(x_{N^*+1}, x_{\ell_2}) \\
& - \overline{D}_{e_2} y(x_{N^*-1}, x_{\ell_2}) \} \overline{D}_\eta v(x_{N^*-1}, x_{\ell_2}) \\
& - \frac{\varepsilon^2}{4} \sum_{\ell_2=N^*}^{N^{**}-1} \nabla_\zeta^2 \phi(\overline{D}_\eta y(x_{N^*-1}, x_{\ell_2-1})) \{ \overline{D}_{e_2} y(x_{N^*+1}, x_{\ell_2}) \\
& - \overline{D}_{e_2} y(x_{N^*-1}, x_{\ell_2}) \} \overline{D}_\eta v(x_{N^*-1}, x_{\ell_2-1}) \\
& - \frac{\varepsilon^2}{4} \sum_{\ell_2=N^*}^{N^{**}-1} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^*-1}, x_{\ell_2})) \{ \overline{D}_{e_2} v(x_{N^*+1}, x_{\ell_2}) \\
& - \overline{D}_{e_2} v(x_{N^*-1}, x_{\ell_2}) \} - \frac{\varepsilon^2}{4} \sum_{\ell_2=N^*}^{N^{**}-1} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^*-1}, x_{\ell_2-1})) \\
& \{ \overline{D}_{e_2} v(x_{N^*+1}, x_{\ell_2}) - \overline{D}_{e_2} v(x_{N^*-1}, x_{\ell_2}) \}.
\end{aligned} \tag{5.74}$$

The first variation of  $E_{2,C_1}$  in the  $e_2$  direction is,

$$\begin{aligned}
\langle DE_{2,C_1}\{y\}, v \rangle_{e_2} = & \frac{\varepsilon^2}{4} \nabla_\zeta^2 \phi(\overline{D}_\eta y(x_{N^*-2}, x_{N^{**}-1})) \{ \overline{D}_{e_2} y(x_{N^*}, x_{N^{**}-1}) \\
& - \overline{D}_{e_2} y(x_{N^*}, x_{N^{**}}) \} \overline{D}_\eta v(x_{N^*-2}, x_{N^{**}-1}) \\
& + \frac{\varepsilon^2}{8} \nabla_\zeta^2 \phi(\overline{D}_\eta y(x_{N^*-1}, x_{N^{**}-1})) \{ \overline{D}_{e_2} y(x_{N^*-1}, x_{N^{**}}) \\
& - \overline{D}_{e_2} y(x_{N^*-1}, x_{N^{**}-1}) \} \overline{D}_\eta v(x_{N^*-1}, x_{N^{**}-1}) \\
& + \frac{\varepsilon^2}{8} \nabla_\zeta^2 \phi(\overline{D}_\eta y(x_{N^*-1}, x_{N^{**}-1})) \{ \overline{D}_{e_2} y(x_{N^*+1}, x_{N^{**}-1}) \\
& - \overline{D}_{e_2} y(x_{N^*+1}, x_{N^{**}}) \} \overline{D}_\eta v(x_{N^*-1}, x_{N^{**}-1}) \\
& + \frac{\varepsilon^2}{4} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^*-2}, x_{N^{**}-1})) \{ \overline{D}_{e_2} v(x_{N^*}, x_{N^{**}-1}) \\
& - \overline{D}_{e_2} v(x_{N^*}, x_{N^{**}}) \} + \frac{\varepsilon^2}{8} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^*-1}, x_{N^{**}-1})) \\
& \{ \overline{D}_{e_2} v(x_{N^*-1}, x_{N^{**}}) - \overline{D}_{e_2} v(x_{N^*-1}, x_{N^{**}-1}) \} \\
& + \frac{\varepsilon^2}{8} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^*-1}, x_{N^{**}-1})) \\
& \{ \overline{D}_{e_2} v(x_{N^*+1}, x_{N^{**}-1}) - \overline{D}_{e_2} v(x_{N^*+1}, x_{N^{**}}) \}.
\end{aligned} \tag{5.75}$$



The first variation of  $E_{2,C_2}$  in the  $e_2$  direction is,

$$\begin{aligned}
\langle DE_{2,C_2}\{y\}, v \rangle_{e_2} = & \frac{\varepsilon^2}{4} \nabla_\zeta^2 \phi(\overline{D}_\eta y(x_{N^{**}-2}, x_{N^{**}-1})) \{ \overline{D}_{e_2} y(x_{N^{**}}, x_{N^{**}}) \\
& - \overline{D}_{e_2} y(x_{N^{**}}, x_{N^{**}-1}) \} \overline{D}_\eta v(x_{N^{**}-2}, x_{N^{**}-1}) \\
& + \frac{\varepsilon^2}{8} \nabla_\zeta^2 \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{N^{**}-1})) \{ \overline{D}_{e_2} y(x_{N^{**}-1}, x_{N^{**}-1}) \\
& - \overline{D}_{e_2} y(x_{N^{**}-1}, x_{N^{**}}) \} \overline{D}_\eta v(x_{N^{**}-1}, x_{N^{**}-1}) \\
& + \frac{\varepsilon^2}{8} \nabla_\zeta^2 \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{N^{**}-1})) \{ \overline{D}_{e_2} y(x_{N^{**}+1}, x_{N^{**}-1}) \\
& - \overline{D}_{e_2} y(x_{N^{**}+1}, x_{N^{**}}) \} \overline{D}_\eta v(x_{N^{**}-1}, x_{N^{**}-1}) \\
& + \frac{\varepsilon^2}{4} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-2}, x_{N^{**}-1})) \{ \overline{D}_{e_2} v(x_{N^{**}}, x_{N^{**}}) \\
& - \overline{D}_{e_2} v(x_{N^{**}}, x_{N^{**}-1}) \} + \frac{\varepsilon^2}{8} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{N^{**}-1})) \\
& \{ \overline{D}_{e_2} v(x_{N^{**}-1}, x_{N^{**}-1}) - \overline{D}_{e_2} v(x_{N^{**}-1}, x_{N^{**}}) \} \\
& + \frac{\varepsilon^2}{8} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{N^{**}-1})) \\
& \{ \overline{D}_{e_2} v(x_{N^{**}+1}, x_{N^{**}-1}) - \overline{D}_{e_2} v(x_{N^{**}+1}, x_{N^{**}}) \}.
\end{aligned} \tag{5.76}$$

The first variation of  $E_{2,C_3}$  in the  $e_2$  direction is,

$$\begin{aligned}
\langle DE_{2,C_3}\{y\}, v \rangle_{e_2} = & \frac{\varepsilon^2}{4} \nabla_\zeta^2 \phi(\overline{D}_\eta y(x_{N^{**}-2}, x_{N^*-1})) \{ \overline{D}_{e_2} y(x_{N^{**}}, x_{N^*-1}) \\
& - \overline{D}_{e_2} y(x_{N^{**}}, x_{N^*}) \} \overline{D}_\eta v(x_{N^{**}-2}, x_{N^*-1}) \\
& + \frac{\varepsilon^2}{8} \nabla_\zeta^2 \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{N^*-1})) \{ \overline{D}_{e_2} y(x_{N^{**}-1}, x_{N^*}) \\
& - \overline{D}_{e_2} y(x_{N^{**}-1}, x_{N^*-1}) \} \overline{D}_\eta v(x_{N^{**}-1}, x_{N^*-1}) \\
& + \frac{\varepsilon^2}{8} \nabla_\zeta^2 \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{N^*-1})) \{ \overline{D}_{e_2} y(x_{N^{**}+1}, x_{N^*-1}) \\
& - \overline{D}_{e_2} y(x_{N^{**}+1}, x_{N^*}) \} \overline{D}_\eta v(x_{N^{**}-1}, x_{N^*-1}) \\
& + \frac{\varepsilon^2}{4} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-2}, x_{N^*-1})) \{ \overline{D}_{e_2} v(x_{N^{**}}, x_{N^*-1}) \\
& - \overline{D}_{e_2} v(x_{N^{**}}, x_{N^*}) \} + \frac{\varepsilon^2}{8} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{N^*-1})) \\
& \{ \overline{D}_{e_2} v(x_{N^{**}-1}, x_{N^*}) - \overline{D}_{e_2} v(x_{N^{**}}, x_{N^*}) \} \\
& + \frac{\varepsilon^2}{8} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{N^*-1})) \\
& \{ \overline{D}_{e_2} v(x_{N^{**}+1}, x_{N^*-1}) - \overline{D}_{e_2} v(x_{N^{**}+1}, x_{N^*}) \}.
\end{aligned} \tag{5.77}$$

The first variation of  $E_{2,C_4}$  in the  $e_2$  direction is,

$$\begin{aligned}
\langle DE_{2,C_4}\{y\}, v \rangle_{e_2} = & \frac{\varepsilon^2}{4} \nabla_\zeta^2 \phi(\overline{D}_\eta y(x_{N^*-2}, x_{N^*-1})) \{ \overline{D}_{e_2} y(x_{N^*}, x_{N^*}) \\
& - \overline{D}_{e_2} y(x_{N^*}, x_{N^*-1}) \} \overline{D}_\eta v(x_{N^*-2}, x_{N^*-1}) \\
& + \frac{\varepsilon^2}{8} \nabla_\zeta^2 \phi(\overline{D}_\eta y(x_{N^*-1}, x_{N^*-1})) \{ \overline{D}_{e_2} y(x_{N^*-1}, x_{N^*-1}) \\
& - \overline{D}_{e_2} y(x_{N^*-1}, x_{N^*}) \} \overline{D}_\eta v(x_{N^*-1}, x_{N^*-1}) \\
& + \frac{\varepsilon^2}{8} \nabla_\zeta^2 \phi(\overline{D}_\eta y(x_{N^*-1}, x_{N^*-1})) \{ \overline{D}_{e_2} y(x_{N^*+1}, x_{N^*}) \\
& - \overline{D}_{e_2} y(x_{N^*+1}, x_{N^*-1}) \} \overline{D}_\eta v(x_{N^*-1}, x_{N^*-1}) \\
& + \frac{\varepsilon^2}{4} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^*-2}, x_{N^*-1})) \{ \overline{D}_{e_2} v(x_{N^*}, x_{N^*}) \\
& - \overline{D}_{e_2} v(x_{N^*}, x_{N^*-1}) \} + \frac{\varepsilon^2}{8} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^*-1}, x_{N^*-1})) \\
& \{ \overline{D}_{e_2} v(x_{N^*-1}, x_{N^*-1}) - \overline{D}_{e_2} v(x_{N^*}, x_{N^*-1}) \} \\
& + \frac{\varepsilon^2}{8} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^*-1}, x_{N^*-1})) \\
& \{ \overline{D}_{e_2} v(x_{N^*+1}, x_{N^*}) - \overline{D}_{e_2} v(x_{N^*+1}, x_{N^*-1}) \}.
\end{aligned} \tag{5.78}$$

#### 5.2.4 Final Calculations

We now subtract the variations (5.71)-(5.78) from the respective calculations (5.62)-(5.69). For interface  $\Gamma_1$ , by subtracting (A.1) from (5.62) we obtain

$$\begin{aligned}
& \frac{\varepsilon^2}{4} \sum_{\ell_1=N^*}^{N^{**}-1} \nabla_\zeta^2 \phi(\overline{D}_\eta y(x_{\ell_1}, x_{N^{**}-1})) \{ \overline{D}_{e_2} y(x_{\ell_1}, x_{N^{**}-1}) \\
& - \overline{D}_{e_2} y(x_{\ell_1}, x_{N^{**}}) \} \overline{D}_\eta v(x_{\ell_1}, x_{N^{**}-1}) \\
& + \frac{\varepsilon^2}{4} \sum_{\ell_1=N^*}^{N^{**}-1} \nabla_\zeta^2 \phi(\overline{D}_\eta y(x_{\ell_1-2}, x_{N^{**}-1})) \{ \overline{D}_{e_2} y(x_{\ell_1}, x_{N^{**}-1}) \\
& - \overline{D}_{e_2} y(x_{\ell_1}, x_{N^{**}}) \} \overline{D}_\eta v(x_{\ell_1-2}, x_{N^{**}-1}),
\end{aligned} \tag{5.79}$$

and similarly for interface  $\Gamma_2$ ,

$$\begin{aligned}
& \varepsilon^2 \sum_{\ell_2=N^*}^{N^{**}-1} \{ -\nabla_\zeta \phi(\nabla y(m_{(N^{**}-1, \ell_2)}) \eta) + \frac{1}{2} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-2}, x_{\ell_2})) \\
& + \frac{1}{2} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^{**}-2}, x_{\ell_2-1})) \} \overline{D}_{e_2} v(x_{N^{**}}, x_{\ell_2}) \\
& + \frac{\varepsilon^2}{4} \sum_{\ell_2=N^*}^{N^{**}-1} \nabla_\zeta^2 \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{\ell_2})) \{ \overline{D}_{e_2} y(x_{N^{**}-1}, x_{\ell_2}) \\
& - \overline{D}_{e_2} y(x_{N^{**}+1}, x_{\ell_2}) \} \overline{D}_\eta v(x_{N^{**}-1}, x_{\ell_2}) \\
& + \frac{\varepsilon^2}{4} \sum_{\ell_2=N^*}^{N^{**}-1} \nabla_\zeta^2 \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{\ell_2-1})) \{ \overline{D}_{e_2} y(x_{N^{**}-1}, x_{\ell_2}) \\
& - \overline{D}_{e_2} y(x_{N^{**}+1}, x_{\ell_2}) \} \overline{D}_\eta v(x_{N^{**}-1}, x_{\ell_2-1}),
\end{aligned} \tag{5.80}$$

for interface  $\Gamma_3$ ,

$$\begin{aligned}
& \frac{\varepsilon^2}{4} \sum_{\ell_1=N^*}^{N^{**}-1} \nabla_\zeta^2 \phi(\overline{D}_\eta y(x_{\ell_1}, x_{N^*-1})) \{ \overline{D}_{e_2} y(x_{\ell_1}, x_{N^*}) \\
& - \overline{D}_{e_2} y(x_{\ell_1}, x_{N^*-1}) \} \overline{D}_\eta v(x_{\ell_1}, x_{N^*-1}) \\
& + \frac{\varepsilon^2}{4} \sum_{\ell_1=N^*}^{N^{**}-1} \nabla_\zeta^2 \phi(\overline{D}_\eta y(x_{\ell_1-2}, x_{N^*-1})) \{ \overline{D}_{e_2} y(x_{\ell_1}, x_{N^*}) \\
& - \overline{D}_{e_2} y(x_{\ell_1}, x_{N^*-1}) \} \overline{D}_\eta v(x_{\ell_1-2}, x_{N^*-1}),
\end{aligned} \tag{5.81}$$

and for interface  $\Gamma_4$ ,

$$\begin{aligned}
& \varepsilon^2 \sum_{\ell_2=N^*}^{N^{**}-1} \{ \nabla_\zeta \phi(\nabla y(m_{(N^*-1, \ell_2)}) \eta) - \frac{1}{2} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^*-2}, x_{\ell_2})) \\
& - \frac{1}{2} \nabla_\zeta \phi(\overline{D}_\eta y(x_{N^*-2}, x_{\ell_2-1})) \} \overline{D}_{e_2} v(x_{N^*}, x_{\ell_2}) \\
& + \frac{\varepsilon^2}{4} \sum_{\ell_2=N^*}^{N^{**}-1} \nabla_\zeta^2 \phi(\overline{D}_\eta y(x_{N^*-1}, x_{\ell_2})) \{ \overline{D}_{e_2} y(x_{N^*+1}, x_{\ell_2}) \\
& - \overline{D}_{e_2} y(x_{N^*-1}, x_{\ell_2}) \} \overline{D}_\eta v(x_{N^*-1}, x_{\ell_2}) \\
& + \frac{\varepsilon^2}{4} \sum_{\ell_2=N^*}^{N^{**}-1} \nabla_\zeta^2 \phi(\overline{D}_\eta y(x_{N^*-1}, x_{\ell_2-1})) \{ \overline{D}_{e_2} y(x_{N^*+1}, x_{\ell_2}) \\
& - \overline{D}_{e_2} y(x_{N^*-1}, x_{\ell_2}) \} \overline{D}_\eta v(x_{N^*-1}, x_{\ell_2-1}).
\end{aligned} \tag{5.82}$$

For corner  $C_1$ , by subtracting (5.75) from (5.66) we obtain

$$\begin{aligned}
& - \frac{\varepsilon^2}{4} \nabla_\zeta^2 \phi(\overline{D}_\eta y(x_{N^*-2}, x_{N^{**}-1})) \{ \overline{D}_{e_2} y(x_{N^*}, x_{N^{**}-1}) \\
& - \overline{D}_{e_2} y(x_{N^*}, x_{N^{**}}) \} \overline{D}_\eta v(x_{N^*-2}, x_{N^{**}-1}) \\
& - \frac{\varepsilon^2}{8} \nabla_\zeta^2 \phi(\overline{D}_\eta y(x_{N^*-1}, x_{N^{**}-1})) \{ \overline{D}_{e_2} y(x_{N^*-1}, x_{N^{**}}) \\
& - \overline{D}_{e_2} y(x_{N^*-1}, x_{N^{**}-1}) \} \overline{D}_\eta v(x_{N^*-1}, x_{N^{**}-1}) \\
& - \frac{\varepsilon^2}{8} \nabla_\zeta^2 \phi(\overline{D}_\eta y(x_{N^*-1}, x_{N^{**}-1})) \{ \overline{D}_{e_2} y(x_{N^*+1}, x_{N^{**}-1}) \\
& - \overline{D}_{e_2} y(x_{N^*+1}, x_{N^{**}}) \} \overline{D}_\eta v(x_{N^*-1}, x_{N^{**}-1}),
\end{aligned} \tag{5.83}$$

and similarly for corner  $C_2$ ,

$$\begin{aligned}
& - \frac{\varepsilon^2}{4} \nabla_\zeta^2 \phi(\overline{D}_\eta y(x_{N^{**}-2}, x_{N^{**}-1})) \{ \overline{D}_{e_2} y(x_{N^{**}}, x_{N^{**}}) \\
& - \overline{D}_{e_2} y(x_{N^{**}}, x_{N^{**}-1}) \} \overline{D}_\eta v(x_{N^{**}-2}, x_{N^{**}-1}) \\
& - \frac{\varepsilon^2}{8} \nabla_\zeta^2 \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{N^{**}-1})) \{ \overline{D}_{e_2} y(x_{N^{**}-1}, x_{N^{**}-1}) \\
& - \overline{D}_{e_2} y(x_{N^{**}-1}, x_{N^{**}}) \} \overline{D}_\eta v(x_{N^{**}-1}, x_{N^{**}-1}) \\
& - \frac{\varepsilon^2}{8} \nabla_\zeta^2 \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{N^{**}-1})) \{ \overline{D}_{e_2} y(x_{N^{**}+1}, x_{N^{**}-1}) \\
& - \overline{D}_{e_2} y(x_{N^{**}+1}, x_{N^{**}}) \} \overline{D}_\eta v(x_{N^{**}-1}, x_{N^{**}-1}),
\end{aligned} \tag{5.84}$$

for corner  $C_3$

$$\begin{aligned}
& -\frac{\varepsilon^2}{4}\nabla_\zeta^2\phi(\overline{D}_\eta y(x_{N^{**}-2}, x_{N^*-1}))\{\overline{D}_{e_2}y(x_{N^{**}}, x_{N^*-1}) \\
& -\overline{D}_{e_2}y(x_{N^{**}}, x_{N^*})\}\overline{D}_\eta v(x_{N^{**}-2}, x_{N^*-1}) \\
& -\frac{\varepsilon^2}{8}\nabla_\zeta^2\phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{N^*-1}))\{\overline{D}_{e_2}y(x_{N^{**}-1}, x_{N^*}) \\
& -\overline{D}_{e_2}y(x_{N^{**}-1}, x_{N^*-1})\}\overline{D}_\eta v(x_{N^{**}-1}, x_{N^*-1}) \\
& -\frac{\varepsilon^2}{8}\nabla_\zeta^2\phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{N^*-1}))\{\overline{D}_{e_2}y(x_{N^{**}+1}, x_{N^*-1}) \\
& -\overline{D}_{e_2}y(x_{N^{**}+1}, x_{N^*})\}\overline{D}_\eta v(x_{N^{**}-1}, x_{N^*-1}),
\end{aligned} \tag{5.85}$$

and for corner  $C_4$

$$\begin{aligned}
& -\frac{\varepsilon^2}{4}\nabla_\zeta^2\phi(\overline{D}_\eta y(x_{N^*-2}, x_{N^*-1}))\{\overline{D}_{e_2}y(x_{N^*}, x_{N^*}) \\
& -\overline{D}_{e_2}y(x_{N^*}, x_{N^*-1})\}\overline{D}_\eta v(x_{N^*-2}, x_{N^*-1}) \\
& -\frac{\varepsilon^2}{8}\nabla_\zeta^2\phi(\overline{D}_\eta y(x_{N^*-1}, x_{N^*-1}))\{\overline{D}_{e_2}y(x_{N^*-1}, x_{N^*-1}) \\
& -\overline{D}_{e_2}y(x_{N^*-1}, x_{N^*})\}\overline{D}_\eta v(x_{N^*-1}, x_{N^*-1}) \\
& -\frac{\varepsilon^2}{8}\nabla_\zeta^2\phi(\overline{D}_\eta y(x_{N^*-1}, x_{N^*-1}))\{\overline{D}_{e_2}y(x_{N^*+1}, x_{N^*}) \\
& -\overline{D}_{e_2}y(x_{N^*+1}, x_{N^*-1})\}\overline{D}_\eta v(x_{N^*-1}, x_{N^*-1}).
\end{aligned} \tag{5.86}$$

If we apply a Taylor expansion as in Chapter 4, Section 4.6.1, we conclude that the order of the remaining terms are  $O(\varepsilon)$ . Similarly, by following the same steps for the  $e_1$  direction for interface  $\Gamma_1$ , we obtain

$$\begin{aligned}
& \varepsilon^2 \sum_{\ell_1=N^*}^{N^{**}-1} \{-\nabla_\zeta\phi(\nabla y(m_{(\ell_1, N^{**}-1)})\eta) + \frac{1}{2}\nabla_\zeta\phi(\overline{D}_\eta y(x_{\ell_1}, x_{N^{**}-2})) \\
& + \frac{1}{2}\nabla_\zeta\phi(\overline{D}_\eta y(x_{\ell_1-1}, x_{N^{**}-2}))\}\overline{D}_{e_1}v(x_{\ell_1}, x_{N^{**}}) \\
& + \frac{\varepsilon^2}{4} \sum_{\ell_1=N^*}^{N^{**}-1} \nabla_\zeta^2\phi(\overline{D}_\eta y(x_{\ell_1}, x_{N^{**}-1}))\{\overline{D}_{e_1}y(x_{\ell_1}, x_{N^{**}+1}) \\
& -\overline{D}_{e_1}y(x_{\ell_1}, x_{N^{**}-1})\}\overline{D}_\eta v(x_{\ell_1-1}, x_{N^{**}-1}) \\
& + \frac{\varepsilon^2}{4} \sum_{\ell_1=N^*}^{N^{**}-1} \nabla_\zeta^2\phi(\overline{D}_\eta y(x_{\ell_1-1}, x_{N^{**}-1}))\{\overline{D}_{e_1}y(x_{\ell_1}, x_{N^{**}+1}) \\
& -\overline{D}_{e_1}y(x_{\ell_1}, x_{N^{**}-1})\}\overline{D}_\eta v(x_{\ell_1-1}, x_{N^{**}-1}),
\end{aligned} \tag{5.87}$$

and similarly for interface  $\Gamma_2$ ,

$$\begin{aligned}
& + \frac{\varepsilon^2}{4} \sum_{\ell_2=N^*}^{N^{**}-1} \nabla_\zeta^2\phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{\ell_2}))\{\overline{D}_{e_1}y(x_{N^{**}-1}, x_{\ell_2}) \\
& -\overline{D}_{e_1}y(x_{N^{**}}, x_{\ell_2})\}\overline{D}_\eta v(x_{N^{**}-1}, x_{\ell_2}) \\
& + \frac{\varepsilon^2}{4} \sum_{\ell_2=N^*}^{N^{**}-1} \nabla_\zeta^2\phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{\ell_2-2}))\{\overline{D}_{e_1}y(x_{N^{**}-1}, x_{\ell_2}) \\
& -\overline{D}_{e_1}y(x_{N^{**}}, x_{\ell_2})\}\overline{D}_\eta v(x_{N^{**}-1}, x_{\ell_2-2}),
\end{aligned} \tag{5.88}$$

for interface  $\Gamma_3$ ,

$$\begin{aligned}
& \varepsilon^2 \sum_{\ell_1=N^*}^{N^{**}-1} \{ \nabla_\zeta \phi(\nabla y(m_{(\ell_1, N^*-1)})\eta) - \frac{1}{2} \nabla_\zeta \phi(\overline{D}_\eta y(x_{\ell_1}, x_{N^*-2})) \\
& \quad - \frac{1}{2} \nabla_\zeta \phi(\overline{D}_\eta y(x_{\ell_1-1}, x_{N^*-2})) \} \overline{D}_{e_1} v(x_{\ell_1}, x_{N^*}) \\
& \quad - \frac{\varepsilon^2}{4} \sum_{\ell_1=N^*}^{N^{**}-1} \nabla_\zeta^2 \phi(\overline{D}_\eta y(x_{\ell_1}, x_{N^*-1})) \{ \overline{D}_{e_1} y(x_{\ell_1}, x_{N^*+1}) \\
& \quad - \overline{D}_{e_1} y(x_{\ell_1}, x_{N^*-1}) \} \overline{D}_\eta v(x_{\ell_1}, x_{N^*-1}) \\
& \quad + \frac{\varepsilon^2}{4} \sum_{\ell_1=N^*}^{N^{**}-1} \nabla_\zeta^2 \phi(\overline{D}_\eta y(x_{\ell_1-1}, x_{N^*-1})) \{ \overline{D}_{e_1} y(x_{\ell_1}, x_{N^*+1}) \\
& \quad - \overline{D}_{e_1} y(x_{\ell_1}, x_{N^*-1}) \} \overline{D}_\eta v(x_{\ell_1-1}, x_{N^*-1}),
\end{aligned} \tag{5.89}$$

and for interface  $\Gamma_4$ ,

$$\begin{aligned}
& \frac{\varepsilon^2}{4} \sum_{\ell_2=N^*}^{N^{**}-1} \nabla_\zeta^2 \phi(\overline{D}_\eta y(x_{N^*-1}, x_{\ell_2})) \{ \overline{D}_{e_1} y(x_{N^*}, x_{\ell_2}) \\
& \quad - \overline{D}_{e_1} y(x_{N^*-1}, x_{\ell_2}) \} \overline{D}_\eta v(x_{N^*-1}, x_{\ell_2}) \\
& \quad + \frac{\varepsilon^2}{4} \sum_{\ell_2=N^*}^{N^{**}-1} \nabla_\zeta^2 \phi(\overline{D}_\eta y(x_{N^*-1}, x_{\ell_2-2})) \{ \overline{D}_{e_1} y(x_{N^*}, x_{\ell_2}) \\
& \quad - \overline{D}_{e_1} y(x_{N^*-1}, x_{\ell_2}) \} \overline{D}_\eta v(x_{N^*-1}, x_{\ell_2-2}).
\end{aligned} \tag{5.90}$$

For corner  $C_1$ , we obtain

$$\begin{aligned}
& - \frac{\varepsilon^2}{4} \nabla_\zeta^2 \phi(\overline{D}_\eta y(x_{N^*-1}, x_{N^{**}-2})) \{ \overline{D}_{e_1} y(x_{N^*-1}, x_{N^{**}}) \\
& \quad - \overline{D}_{e_1} y(x_{N^*}, x_{N^{**}}) \} \overline{D}_\eta v(x_{N^*-1}, x_{N^{**}-2}) \\
& \quad - \frac{\varepsilon^2}{8} \nabla_\zeta^2 \phi(\overline{D}_\eta y(x_{N^*-1}, x_{N^{**}-1})) \{ \overline{D}_{e_1} y(x_{N^*}, x_{N^{**}-1}) \\
& \quad - \overline{D}_{e_1} y(x_{N^*}, x_{N^{**}+1}) \} \overline{D}_\eta v(x_{N^*-1}, x_{N^{**}-1}) \\
& \quad - \frac{\varepsilon^2}{8} \nabla_\zeta^2 \phi(\overline{D}_\eta y(x_{N^*-1}, x_{N^{**}+1})) \{ \overline{D}_{e_1} y(x_{N^*-1}, x_{N^{**}+1}) \\
& \quad - \overline{D}_{e_1} y(x_{N^*-1}, x_{N^{**}-1}) \} \overline{D}_\eta v(x_{N^*-1}, x_{N^{**}-1}),
\end{aligned} \tag{5.91}$$

and similarly for corner  $C_2$ ,

$$\begin{aligned}
& - \frac{\varepsilon^2}{4} \nabla_\zeta^2 \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{N^{**}-2})) \{ \overline{D}_{e_1} y(x_{N^{**}}, x_{N^{**}}) \\
& \quad - \overline{D}_{e_1} y(x_{N^{**}-1}, x_{N^{**}}) \} \overline{D}_\eta v(x_{N^{**}-1}, x_{N^{**}-2}) \\
& \quad - \frac{\varepsilon^2}{8} \nabla_\zeta^2 \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{N^{**}-1})) \{ \overline{D}_{e_1} y(x_{N^{**}-1}, x_{N^{**}-1}) \\
& \quad - \overline{D}_{e_1} y(x_{N^{**}-1}, x_{N^{**}+1}) \} \overline{D}_\eta v(x_{N^{**}-1}, x_{N^{**}-1}) \\
& \quad - \frac{\varepsilon^2}{8} \nabla_\zeta^2 \phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{N^{**}+1})) \{ \overline{D}_{e_1} y(x_{N^{**}}, x_{N^{**}+1}) \\
& \quad - \overline{D}_{e_1} y(x_{N^{**}}, x_{N^{**}-1}) \} \overline{D}_\eta v(x_{N^{**}-1}, x_{N^{**}-1}),
\end{aligned} \tag{5.92}$$

for corner  $C_3$

$$\begin{aligned}
& -\frac{\varepsilon^2}{4}\nabla_\zeta^2\phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{N^*-2}))\{\overline{D}_{e_1}y(x_{N^{**}-1}, x_{N^*}) \\
& -\overline{D}_{e_1}y(x_{N^{**}}, x_{N^*})\}\overline{D}_\eta v(x_{N^{**}-1}, x_{N^*-2}) \\
& -\frac{\varepsilon^2}{8}\nabla_\zeta^2\phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{N^*-1,2}))\{\overline{D}_{e_1}y(x_{N^{**}-1}, x_{N^*}) \\
& -\overline{D}_{e_1}y(x_{N^{**}}, x_{N^*})\}\overline{D}_\eta v(x_{N^{**}-1}, x_{N^*-2}) \\
& -\frac{\varepsilon^2}{8}\nabla_\zeta^2\phi(\overline{D}_\eta y(x_{N^{**}-1}, x_{N^*-1}))\{\overline{D}_{e_1}y(x_{N^{**}}, x_{N^*-1}) \\
& -\overline{D}_{e_1}y(x_{N^{**}-1}, x_{N^*-1})\}\overline{D}_\eta v(x_{N^{**}-1}, x_{N^*-1}),
\end{aligned} \tag{5.93}$$

and for corner  $C_4$

$$\begin{aligned}
& -\frac{\varepsilon^2}{4}\nabla_\zeta^2\phi(\overline{D}_\eta y(x_{N^*-1}, x_{N^*-2}))\{\overline{D}_{e_1}y(x_{N^*}, x_{N^*}) \\
& -\overline{D}_{e_1}y(x_{N^*-1}, x_{N^*})\}\overline{D}_\eta v(x_{N^*-1}, x_{N^*-2}) \\
& -\frac{\varepsilon^2}{8}\nabla_\zeta^2\phi(\overline{D}_\eta y(x_{N^*-1}, x_{N^*-1}))\{\overline{D}_{e_1}y(x_{N^*}, x_{N^*+1}) \\
& -\overline{D}_{e_1}y(x_{N^*-1}, x_{N^*+1})\}\overline{D}_\eta v(x_{N^*-1}, x_{N^*-1}) \\
& -\frac{\varepsilon^2}{8}\nabla_\zeta^2\phi(\overline{D}_\eta y(x_{N^*-1}, x_{N^*-1}))\{\overline{D}_{e_1}y(x_{N^*-1}, x_{N^*-1}) \\
& -\overline{D}_{e_1}y(x_{N^*}, x_{N^*-1})\}\overline{D}_\eta v(x_{N^*-1}, x_{N^*-1}).
\end{aligned} \tag{5.94}$$

Again, if a Taylor expansion is applied as mentioned earlier on in this section, we conclude that the order of the remaining terms are  $O(\varepsilon)$ . We are ready therefore to prove the main result of this chapter.

**Theorem 6.** (VARIATIONAL ERROR) *Let  $y$  be a smooth function; then, for any  $v \in \mathbb{V}_{\varepsilon,Q}$ , the atomistic variation  $\langle D\Phi^{CB}(y), v \rangle$  approximates the variation of the coupled discontinuous method  $\langle D\mathcal{E}_2^D\{y\}, v \rangle$  in the sense that there exist a constant  $M_V = M_V(y, p)$ ,  $1 \leq p \leq \infty$ , independent of  $v$ , such that*

$$\left| \langle D\mathcal{E}_2^D\{y\}, v \rangle - \langle D\Phi^{CB}(y), v \rangle_\varepsilon \right| \leq M_V (\varepsilon^2 + \varepsilon^{2-1/p}) |v|_{W^{1,p}(\Omega)}.$$

*Proof.* The proof is similar to the one dimensional result in Chapter 3, so the details are omitted. Collecting the results in this chapter we observe that

$$\begin{aligned}
\langle D\Phi_2^{CB}(y) - D\mathcal{E}_2^D(y), v \rangle_\varepsilon &= \varepsilon^2 \sum_{\ell \in \mathcal{L} \setminus S_\Gamma} \alpha_\ell [\overline{D}_{e_1}v_\ell + \overline{D}_{e_2}v_\ell] \\
&+ \varepsilon^2 \sum_{\ell \in S_\Gamma} \beta_\ell [\overline{D}_{e_1}v_\ell + \overline{D}_{e_2}v_\ell],
\end{aligned} \tag{5.95}$$

where  $\alpha_\ell = \mathcal{O}(\varepsilon^2)$ ,  $\beta_\ell = \mathcal{O}(\varepsilon)$  and  $S_\Gamma$  is the collection of the interface indices. As in

Chapter 4,  $\sum_{\ell \in S_\Gamma} 1 = \mathcal{O}(1/\varepsilon)$  and hence  $(1/p + 1/q = 1)$ ,

$$\begin{aligned}
& |\langle D\Phi_2^{CB}(y) - D\mathcal{E}_2^D(y), v \rangle_\varepsilon | \\
& \leq C \left( \varepsilon^2 \sum_{\ell \in \mathcal{L} \setminus S_\Gamma} |\alpha_\ell|^q + \varepsilon^2 \sum_{\ell \in S_\Gamma} |\beta_\ell|^q \right)^{1/q} \left( \varepsilon^2 \sum_{\ell=1}^N |\overline{D}_{e_1} v_\ell + \overline{D}_{e_2} v_\ell|^p \right)^{1/p} \\
& \leq C \left( \varepsilon^2 \sum_{\ell \in \mathcal{L} \setminus S_\Gamma} |\alpha_\ell|^q + \varepsilon^2 \sum_{\ell \in S_\Gamma} |\beta_\ell|^q \right)^{1/q} |v|_{W^{1,p}(\Omega)},
\end{aligned} \tag{5.96}$$

where in the last bound we have used that  $v \in \mathbb{V}_{\varepsilon,Q}$ . Now

$$\begin{aligned}
\left( \varepsilon^2 \sum_{\ell \in \mathcal{L} \setminus S_\Gamma} |\alpha_\ell|^q + \varepsilon^2 \sum_{\ell \in S_\Gamma} |\beta_\ell|^q \right)^{1/q} & \leq C \left( |\Omega| \varepsilon^{2q} + |\Gamma| \varepsilon^{q+1} \right)^{1/q} \\
& \leq C(\varepsilon^2 + \varepsilon^{(q+1)/q}),
\end{aligned} \tag{5.97}$$

and the result follows since  $(q+1)/q = 2 - 1/p$ .  $\square$

# Chapter 6

## The Three Body Problem

### 6.1 Chapter Overview

The results of the previous chapters were devoted to pair potentials. The extension of the design and analysis of consistent methods to multi-body potentials is quite challenging and requires new ideas. Initial results in this direction can be found in [25]. A three body atomistic potential can be written as,

$$\Phi_3^a(y) := \varepsilon^2 \sum_{\ell \in \mathcal{L}} \sum_{\eta, \eta' \in R} \phi(\overline{D}_\eta y_\ell, \overline{D}_{\eta'} y_\ell), \quad (6.1)$$

i.e., the local interatomic potential  $\phi = \phi_3$  is a function of both  $\overline{D}_\eta y_\ell$ , and  $\overline{D}_{\eta'} y_\ell$ . In this chapter we extend the energy consistency result of [21] to multi-body potentials. The results below are the first consistency results in the literature for three-body potentials using atomistic Cauchy-Born models and finite element tools. As will become evident in the proof, the creation of new symmetries is required as well as the need to assume standard symmetry hypotheses for the potential. The corresponding Cauchy-Born stored energy function is

$$W_{CB}(F) = W_{3,CB}(F) := \sum_{\eta, \eta' \in R} \phi(F\eta, F\eta') \quad (6.2)$$

and

$$\Phi^{CB}(y) := \int_{\Omega} W_{CB}(\nabla y(x)) dx. \quad (6.3)$$

In Section 6.2 we state and prove three lemmas that are needed to prove the theorem in the next section. In Section 6.3 we prove Theorem 7 that states that for a smooth function  $y$  and an interatomic potential  $\phi$  that is both Lipschitz continuous and satisfies the symmetry property

$$\phi(\overline{D}_\eta y_\ell, \overline{D}_{\eta'} y_\ell) = \phi(-\overline{D}_{-\eta} y_\ell, -\overline{D}_{-\eta'} y_\ell), \quad (6.4)$$

the Cauchy-Born continuum energy is a second order approximation to the atomistic energy  $\Phi^a(y)$  where there exists a constant  $M_E = M_E(y)$  such that

$$\left| \Phi^{CB}(y) - \Phi_3^a(y) \right| \leq M_E \varepsilon^2. \quad (6.5)$$

Notice that the above symmetry assumption is quite natural from a physical perspective, and a typical hypothesis in the analysis of atomistic models in the bibliography.



## 6.2 Lemmas for the Three Body Problem

In this section three lemmas will be stated and proved in order to be able to prove the main theorem for the three body problem in the next section.

**Lemma 24.** *For a smooth function  $y$  and an interatomic potential that satisfies the symmetry property*

$$\phi(\bar{D}_\eta y_\ell, \bar{D}_{\eta'} y_\ell) = \phi(-\bar{D}_{-\eta} y_\ell, -\bar{D}_{-\eta'} y_\ell), \quad (6.6)$$

*the following bound holds*

$$\begin{aligned} & \left| \frac{\varepsilon^2}{2} \sum_{\ell \in \mathcal{L}} \sum_{\eta, \eta' \in R} \phi(\bar{D}_\eta y_\ell, \bar{D}_{\eta'} y_\ell) + \frac{\varepsilon^2}{2} \sum_{\ell \in \mathcal{L}} \sum_{\eta, \eta' \in R} \phi(-\bar{D}_{-\eta} y_\ell, -\bar{D}_{-\eta'} y_\ell) - \right. \\ & \left. \varepsilon^2 \sum_{\ell \in \mathcal{L}} \sum_{\eta, \eta' \in R} \phi\left(\frac{\bar{D}_\eta y_\ell - \bar{D}_{-\eta} y_\ell}{2}, \frac{\bar{D}_{\eta'} y_\ell - \bar{D}_{-\eta'} y_\ell}{2}\right) \right| \leq C \varepsilon^2. \end{aligned} \quad (6.7)$$

*Proof.* Due to the symmetry property the three body atomistic potential can be expressed as

$$\begin{aligned} \frac{\varepsilon^2}{2} \sum_{\ell \in \mathcal{L}} \sum_{\eta, \eta' \in R} \phi(\bar{D}_\eta y_\ell, \bar{D}_{\eta'} y_\ell) &= \frac{\varepsilon^2}{2} \sum_{\ell \in \mathcal{L}} \sum_{\eta, \eta' \in R} \phi(\bar{D}_\eta y_\ell, \bar{D}_{\eta'} y_\ell) \\ &+ \frac{\varepsilon^2}{2} \sum_{\ell \in \mathcal{L}} \sum_{\eta, \eta' \in R} \phi(-\bar{D}_{-\eta} y_\ell, -\bar{D}_{-\eta'} y_\ell). \end{aligned} \quad (6.8)$$

Let function  $\phi : \mathbb{R}^n \rightarrow \mathbb{R}$  be  $k$  times differentiable at the point  $\alpha \in \mathbb{R}^n$  such that the multivariate Taylor theorem can be applied. It is a simple matter to verify that

$$\begin{aligned} \phi(x_1, y_1) + \phi(x_2, y_2) &= 2\phi\left(\frac{x_1 + x_2}{2}, \frac{y_1 + y_2}{2}\right) \\ &+ \left[ \frac{\partial^2 \phi}{\partial x^2} \left(\frac{x_1 + x_2}{2}, \frac{y_1 + y_2}{2}\right) \left(\frac{x_2 - x_1}{2}\right)^2 \right. \\ &+ 2 \frac{\partial^2 \phi}{\partial x \partial y} \left(\frac{x_1 + x_2}{2}, \frac{y_1 + y_2}{2}\right) \left(\frac{x_2 - x_1}{2} \frac{y_2 - y_1}{2}\right) \\ &\left. + \frac{\partial^2 \phi}{\partial y^2} \left(\frac{x_1 + x_2}{2}, \frac{y_1 + y_2}{2}\right) \left(\frac{y_2 - y_1}{2}\right)^2 \right] + \mathcal{O}\left(\frac{x_2 - x_1}{2}, \frac{y_2 - y_1}{2}\right)^3, \end{aligned} \quad (6.9)$$

By implementing this Taylor series expansion to (6.8) yields

$$\begin{aligned} & \left| \frac{\varepsilon^2}{2} \sum_{\ell \in \mathcal{L}} \sum_{\eta, \eta' \in R} \phi(\bar{D}_\eta y_\ell, \bar{D}_{\eta'} y_\ell) + \frac{\varepsilon^2}{2} \sum_{\ell \in \mathcal{L}} \sum_{\eta, \eta' \in R} \phi(-\bar{D}_{-\eta} y_\ell, -\bar{D}_{-\eta'} y_\ell) - \right. \\ & \left. \varepsilon^2 \sum_{\ell \in \mathcal{L}} \sum_{\eta, \eta' \in R} \phi\left(\frac{\bar{D}_\eta y_\ell - \bar{D}_{-\eta} y_\ell}{2}, \frac{\bar{D}_{\eta'} y_\ell - \bar{D}_{-\eta'} y_\ell}{2}\right) \right| \leq \\ & \left| \frac{\partial^2 \phi}{\partial x^2} \left(\frac{\bar{D}_\eta y_\ell - \bar{D}_{-\eta} y_\ell}{2}, \frac{\bar{D}_{\eta'} y_\ell - \bar{D}_{-\eta'} y_\ell}{2}\right) \right| \left| \frac{-\bar{D}_{-\eta} y_\ell - \bar{D}_\eta y_\ell}{2} \right|^2 + \\ & 2 \left| \frac{\partial^2 \phi}{\partial x \partial y} \left(\frac{\bar{D}_\eta y_\ell - \bar{D}_{-\eta} y_\ell}{2}, \frac{\bar{D}_{\eta'} y_\ell - \bar{D}_{-\eta'} y_\ell}{2}\right) \right| \left| \frac{-\bar{D}_{-\eta} y_\ell - \bar{D}_\eta y_\ell}{2} \frac{-\bar{D}_{-\eta'} y_\ell - \bar{D}_{\eta'} y_\ell}{2} \right| + \\ & \left| \frac{\partial^2 \phi}{\partial y^2} \left(\frac{\bar{D}_\eta y_\ell - \bar{D}_{-\eta} y_\ell}{2}, \frac{\bar{D}_{\eta'} y_\ell - \bar{D}_{-\eta'} y_\ell}{2}\right) \right| \left| \frac{-\bar{D}_{-\eta'} y_\ell - \bar{D}_{\eta'} y_\ell}{2} \right|^2 + R_1, \end{aligned} \quad (6.10)$$

where the remainder term  $R_1$  accounts for the last term in (6.9). We just need to show that

$$\left| \frac{-\bar{D}_{-\eta}y_\ell - \bar{D}_\eta y_\ell}{2} \right| \leq \mathcal{O}(\varepsilon), \quad (6.11)$$

and

$$\left| \frac{-\bar{D}_{-\eta'}y_\ell - \bar{D}_{\eta'}y_\ell}{2} \right| \leq \mathcal{O}(\varepsilon), \quad (6.12)$$

for (6.7) to hold. Considering (6.11), we note that

$$\begin{aligned} \frac{-\bar{D}_{-\eta}y_\ell - \bar{D}_\eta y_\ell}{2} &= \left\{ \frac{1}{2}\bar{D}_{\eta_1 e_1}y_{\ell-\eta} + \frac{1}{2}\bar{D}_{\eta_2 e_2}y_{\ell-\eta_2 e_2} \right\} + \left\{ \frac{1}{2}\bar{D}_{\eta_2 e_2}y_{\ell-\eta} + \frac{1}{2}\bar{D}_{\eta_1 e_1}y_{\ell-\eta_1 e_1} \right\} \\ &\quad - \left\{ \frac{1}{2}\bar{D}_{\eta_1 e_1}y_\ell + \frac{1}{2}\bar{D}_{\eta_1 e_1}y_{\ell+\eta_2 e_2} \right\} - \left\{ \frac{1}{2}\bar{D}_{\eta_2 e_2}y_\ell + \frac{1}{2}\bar{D}_{\eta_2 e_2}y_{\ell+\eta_1 e_1} \right\} \\ &= \frac{1}{2\varepsilon} \{ y_{\ell-\eta_2 e_2} - y_{\ell-\eta} + y_\ell - y_{\ell-\eta_2 e_2} + y_{\ell-\eta_1 e_1} - y_{\ell-\eta} + y_\ell - y_{\ell-\eta_1 e_1} \} \\ &\quad - \frac{1}{2\varepsilon} \{ y_{\ell+\eta_1 e_1} - y_\ell + y_{\ell+\eta} - y_{\ell+\eta_2 e_2} + y_{\ell+\eta_2 e_2} - y_\ell + y_{\ell+\eta} \\ &\quad - y_{\ell+\eta_1 e_1} \}. \end{aligned} \quad (6.13)$$

Then the desired result follows by observing, for example,

$$\frac{y_{\ell-\eta_2 e_2} - y_{\ell-\eta}}{\varepsilon} = \eta_2 \frac{y_{\ell-\eta_2 e_2} - y_\ell}{\eta_2 \varepsilon} = \eta_2 \frac{\partial y_\ell}{\partial x_2} + \mathcal{O}(\varepsilon), \quad (6.14)$$

and applying Taylor's formula.  $\square$

By applying the same steps, the following estimate also holds

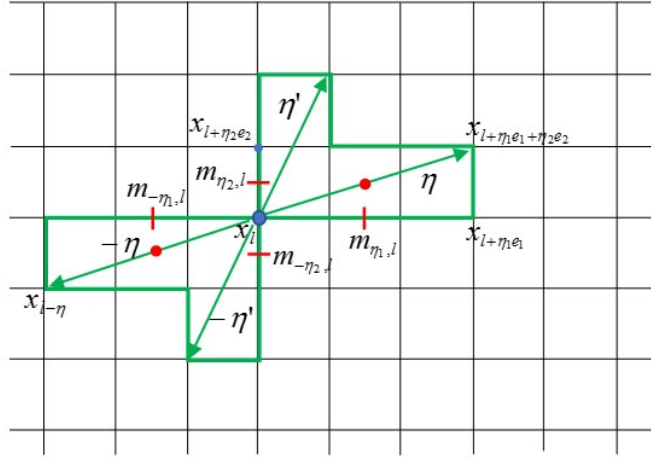
$$\begin{aligned} &\left| \frac{\varepsilon^2}{2} \sum_{\ell \in \mathcal{L}} \sum_{\eta, \eta' \in R} \phi(\bar{D}_\eta y_{\ell+e_1+e_2}, \bar{D}_{\eta'} y_{\ell+e_1+e_2}) \right. \\ &\quad + \frac{\varepsilon^2}{2} \sum_{\ell \in \mathcal{L}} \sum_{\eta, \eta' \in R} \phi(-\bar{D}_{-\eta} y_{\ell+e_1+e_2}, -\bar{D}_{-\eta'} y_{\ell+e_1+e_2}) \\ &\quad \left. - \varepsilon^2 \sum_{\ell \in \mathcal{L}} \sum_{\eta, \eta' \in R} \phi\left( \frac{\bar{D}_\eta y_{\ell+e_1+e_2} - \bar{D}_{-\eta} y_{\ell+e_1+e_2}}{2}, \frac{\bar{D}_{\eta'} y_{\ell+e_1+e_2} - \bar{D}_{-\eta'} y_{\ell+e_1+e_2}}{2} \right) \right| \leq C \varepsilon^2. \end{aligned} \quad (6.15)$$

**Lemma 25.** *Under standard smoothness assumptions on  $y$  we have*

$$\left| \frac{\bar{D}_\eta y_\ell - \bar{D}_{-\eta} y_\ell}{2} - \nabla y(x_\ell) \eta \right| \leq C \varepsilon^2, \quad (6.16)$$

and similarly,

$$\left| \frac{\bar{D}_{\eta'} y_\ell - \bar{D}_{-\eta'} y_\ell}{2} - \nabla y(x_\ell) \eta' \right| \leq C \varepsilon^2. \quad (6.17)$$



**Figure 6.1:** Displaying  $m_{\eta_1, \ell}$ ,  $m_{-\eta_1, \ell}$ ,  $m_{\eta_2, \ell}$  and  $m_{-\eta_2, \ell}$

*Proof.* We will focus on (6.16) and prove the inequality. We note that

$$\begin{aligned}
 \frac{(\overline{D}_\eta y_\ell - \overline{D}_{-\eta} y_\ell)}{2} &= \frac{1}{2} \left\{ \frac{1}{2} \overline{D}_{\eta_1 e_1} y_\ell + \frac{1}{2} \overline{D}_{\eta_2 e_2} y_{\ell + \eta_1 e_1} \right\} + \frac{1}{2} \left\{ \frac{1}{2} \overline{D}_{\eta_2 e_2} y_\ell + \frac{1}{2} \overline{D}_{\eta_1 e_1} y_{\ell + \eta_2 e_2} \right\} \\
 &\quad + \frac{1}{2} \left\{ \frac{1}{2} \overline{D}_{\eta_1 e_1} y_{\ell - \eta} + \frac{1}{2} \overline{D}_{\eta_2 e_2} y_{\ell - \eta_2 e_2} \right\} + \frac{1}{2} \left\{ \frac{1}{2} \overline{D}_{\eta_2 e_2} y_{\ell - \eta} \right. \\
 &\quad \left. + \frac{1}{2} \overline{D}_{\eta_1 e_1} y_{\ell - \eta_1 e_1} \right\}.
 \end{aligned} \tag{6.18}$$

Let us denote

- $m_{\eta_1, \ell}$  to be the midpoint of the side with endpoints  $x_\ell, x_{\ell + \eta_1 e_1}$
- $m_{-\eta_1, \ell}$  to be the midpoint of the side with endpoints  $x_{\ell - \eta_1 e_1}, x_\ell$
- $m_{\eta_2, \ell}$  to be the midpoint of the side with endpoints  $x_\ell, x_{\ell + \eta_2 e_2}$
- $m_{-\eta_2, \ell}$  to be the midpoint of the side with endpoints  $x_{\ell - \eta_2 e_2}, x_\ell$

which are all displayed in Figure 6.1. By combining the terms in (6.18) in a different

order and using symmetries around the midpoints defined above, we obtain

$$\begin{aligned}
\frac{1}{2}\overline{D}_{\eta_2 e_2} y_\ell + \frac{1}{2}\overline{D}_{\eta_2 e_2} y_{\ell+\eta_1 e_1} &= \frac{1}{2} \frac{(y_{\ell+\eta_2 e_2} - y_\ell)}{\varepsilon} + \frac{1}{2} \frac{(y_{\ell+\eta} - y_{\ell+\eta_1 e_1})}{\varepsilon} \\
&= \frac{1}{2} \frac{(y(x_{\ell_1}, x_{\ell_2+\eta_2}) - y(x_{\ell_1}, x_{\ell_2}))}{\varepsilon} \\
&\quad + \frac{1}{2} \frac{(y(x_{\ell_1+\eta_1}, x_{\ell_2+\eta_2}) - y(x_{\ell_1+\eta_1}, x_{\ell_2}))}{\varepsilon} \\
&= \frac{1}{2\varepsilon} \int_{x_{\ell_2}}^{x_{\ell_2+\eta_2}} \left[ \frac{\partial y}{\partial x_2}(x_{\ell_1}, s) + \frac{\partial y}{\partial x_2}(x_{\ell_1+\eta_1}, s) \right] ds \\
&= \frac{1}{\varepsilon} \int_{x_{\ell_2}}^{x_{\ell_2+\eta_2}} \frac{\partial}{\partial x_2} y(m_{\eta_1, \ell}, s) ds + \mathcal{O}(\varepsilon^2) \\
&= \frac{1}{\varepsilon} \int_{x_{\ell_2}}^{x_{\ell_2+\eta_2}} \frac{\partial}{\partial x_2} y(m_{\eta_1, \ell}, m_{\eta_2, \ell}) ds + \mathcal{O}(\varepsilon^2) \\
&= \eta_2 \frac{\partial}{\partial x_2} y(m_{\eta_1, \ell}, m_{\eta_2, \ell}) + \mathcal{O}(\varepsilon^2).
\end{aligned} \tag{6.19}$$

Similarly,

$$\begin{aligned}
\frac{1}{2}\overline{D}_{\eta_1 e_1} y_{\ell+\eta_2 e_2} + \frac{1}{2}\overline{D}_{\eta_1 e_1} y_\ell &= \frac{1}{2} \frac{(y_{\ell+\eta} - y_{\ell+\eta_2 e_2})}{\varepsilon} + \frac{1}{2} \frac{(y_{\ell+\eta_1 e_1} - y_\ell)}{\varepsilon} \\
&= \frac{1}{2} \frac{(y(x_{\ell_1+\eta_1}, x_{\ell_2+\eta_2}) - y(x_{\ell_1}, x_{\ell_2+\eta_2}))}{\varepsilon} \\
&\quad + \frac{1}{2} \frac{(y(x_{\ell_1+\eta_1}, x_{\ell_2}) - y(x_{\ell_1}, x_{\ell_2}))}{\varepsilon} \\
&= \frac{1}{2\varepsilon} \int_{x_{\ell_1}}^{x_{\ell_1+\eta_1}} \left[ \frac{\partial y}{\partial x_1}(s, x_{\ell_2+\eta_2}) + \frac{\partial y}{\partial x_1}(s, x_{\ell_2}) \right] ds \\
&= \frac{1}{\varepsilon} \int_{x_{\ell_1}}^{x_{\ell_1+\eta_1}} \frac{\partial}{\partial x_1} y(s, m_{\eta_2, \ell}) ds + \mathcal{O}(\varepsilon^2) \\
&= \frac{1}{\varepsilon} \int_{x_{\ell_1}}^{x_{\ell_1+\eta_1}} \frac{\partial}{\partial x_1} y(m_{\eta_1, \ell}, m_{\eta_2, \ell}) ds + \mathcal{O}(\varepsilon^2) \\
&= \eta_1 \frac{\partial}{\partial x_1} y(m_{\eta_1, \ell}, m_{\eta_2, \ell}) + \mathcal{O}(\varepsilon^2),
\end{aligned} \tag{6.20}$$

and

$$\begin{aligned}
\frac{1}{2}\overline{D}_{\eta_2 e_2} y_{\ell-\eta} + \frac{1}{2}\overline{D}_{\eta_2 e_2} y_{\ell-\eta_2 e_2} &= \frac{1}{2} \frac{(y_{\ell-\eta_1 e_1} - y_{\ell-\eta_1 e_1 - \eta_2 e_2})}{\varepsilon} + \frac{1}{2} \frac{(y_{\ell} - y_{\ell-\eta_2 e_2})}{\varepsilon} \\
&= \frac{1}{2} \frac{(y(x_{\ell_1-\eta_1}, x_{\ell_2}) - y(x_{\ell_1-\eta_1}, x_{\ell_2-\eta_2}))}{\varepsilon} \\
&\quad + \frac{1}{2} \frac{(y(x_{\ell_1}, x_{\ell_2}) - y(x_{\ell_1}, x_{\ell_2-\eta_2}))}{\varepsilon} \\
&= \frac{1}{2\varepsilon} \int_{x_{\ell_2-\eta_2}}^{x_{\ell_2}} \left[ \frac{\partial y}{\partial x_2}(x_{\ell_1-\eta_1}, s) + \frac{\partial y}{\partial x_2}(x_{\ell_1}, s) \right] ds \\
&= \frac{1}{\varepsilon} \int_{x_{\ell_2-\eta_2}}^{x_{\ell_2}} \frac{\partial}{\partial x_2} y(m_{-\eta_1, \ell}, s) ds + \mathcal{O}(\varepsilon^2) \\
&= \frac{1}{\varepsilon} \int_{x_{\ell_2-\eta_2}}^{x_{\ell_2}} \frac{\partial v}{\partial x_2} y(m_{-\eta_1, \ell}, m_{-\eta_2, \ell}) ds + \mathcal{O}(\varepsilon^2) \\
&= \eta_2 \frac{\partial}{\partial x_2} y(m_{-\eta_1, \ell}, m_{-\eta_2, \ell}) + \mathcal{O}(\varepsilon^2),
\end{aligned} \tag{6.21}$$

and finally

$$\begin{aligned}
\frac{1}{2}\overline{D}_{\eta_1 e_1} y_{\ell-\eta_1 e_1} + \frac{1}{2}\overline{D}_{\eta_1 e_1} y_{\ell-\eta} &= \frac{1}{2} \frac{(y_{\ell} - y_{\ell-\eta_1 e_1})}{\varepsilon} + \frac{1}{2} \frac{(y_{\ell-\eta_2 e_2} - y_{\ell-\eta})}{\varepsilon} \\
&= \frac{1}{2} \frac{(y(x_{\ell_1}, x_{\ell_2}) - y(x_{\ell_1-\eta_1}, x_{\ell_2}))}{\varepsilon} \\
&\quad + \frac{1}{2} \frac{(y(x_{\ell_1}, x_{\ell_2-\eta_2}) - y(x_{\ell_1-\eta_1}, x_{\ell_2-\eta_2}))}{\varepsilon} \\
&= \frac{1}{2\varepsilon} \int_{x_{\ell_1-\eta_1}}^{x_{\ell_1}} \left[ \frac{\partial y}{\partial x_1}(s, x_{\ell_2}) + \frac{\partial y}{\partial x_1}(s, x_{\ell_2-\eta_2}) \right] ds \\
&= \frac{1}{\varepsilon} \int_{x_{\ell_1-\eta_1}}^{x_{\ell_1}} \frac{\partial}{\partial x_1} y(s, m_{-\eta_2, \ell}) ds + \mathcal{O}(\varepsilon^2) \\
&= \frac{1}{\varepsilon} \int_{x_{\ell_1-\eta_1}}^{x_{\ell_1}} \frac{\partial y}{\partial x_1} y(m_{-\eta_1, \ell}, m_{-\eta_2, \ell}) ds + \mathcal{O}(\varepsilon^2) \\
&= \eta_1 \frac{\partial}{\partial x_1} y(m_{-\eta_1, \ell}, m_{-\eta_2, \ell}) + \mathcal{O}(\varepsilon^2).
\end{aligned} \tag{6.22}$$

By substituting (6.19)-(6.22) into (6.18) we obtain

$$\begin{aligned}
\frac{(\overline{D}_{\eta} y_{\ell} - \overline{D}_{-\eta} y_{\ell})}{2} &= \frac{\eta_2}{2} \frac{\partial}{\partial x_2} y(m_{\eta_1, \ell}, m_{\eta_2, \ell}) + \frac{\eta_1}{2} \frac{\partial}{\partial x_1} y(m_{\eta_1, \ell}, m_{\eta_2, \ell}) \\
&\quad + \frac{\eta_2}{2} \frac{\partial}{\partial x_2} y(m_{-\eta_1, \ell}, m_{-\eta_2, \ell}) + \frac{\eta_1}{2} \frac{\partial}{\partial x_1} y(m_{-\eta_1, \ell}, m_{-\eta_2, \ell}) + \mathcal{O}(\varepsilon^2).
\end{aligned} \tag{6.23}$$

By applying Taylor expansion to each term in (6.23) separately we obtain

$$\begin{aligned}
\frac{\partial}{\partial x_1} y(m_{\eta_1, \ell}, m_{\eta_2, \ell}) &= \frac{\partial}{\partial x_1} y\left(\frac{m_{\eta_1, \ell} + m_{-\eta_1, \ell}}{2}, \frac{m_{\eta_2, \ell} + m_{-\eta_2, \ell}}{2}\right) \\
&\quad + \frac{\partial^2}{\partial x_1^2} y\left(\frac{m_{\eta_1, \ell} + m_{-\eta_1, \ell}}{2}, \frac{m_{\eta_2, \ell} + m_{-\eta_2, \ell}}{2}\right) \left(\frac{x_{\ell_1 + \eta_1 e_1} - x_{\ell_1}}{2}\right) \\
&\quad + \frac{\partial^2}{\partial x_1 \partial x_2} y\left(\frac{m_{\eta_1, \ell} + m_{-\eta_1, \ell}}{2}, \frac{m_{\eta_2, \ell} + m_{-\eta_2, \ell}}{2}\right) \left(\frac{x_{\ell_2 + \eta_2 e_2} - x_{\ell_2}}{2}\right) \\
&\quad + \mathcal{O}\left(\frac{x_{\ell_2 + \eta_2 e_2} - x_{\ell_2}}{2}, \frac{x_{\ell_1 + \eta_1 e_1} - x_{\ell_1}}{2}\right)^2,
\end{aligned} \tag{6.24}$$

and

$$\begin{aligned}
\frac{\partial}{\partial x_1} y(m_{-\eta_1, \ell}, m_{-\eta_2, \ell}) &= \frac{\partial}{\partial x_1} y\left(\frac{m_{\eta_1, \ell} + m_{-\eta_1, \ell}}{2}, \frac{m_{\eta_2, \ell} + m_{-\eta_2, \ell}}{2}\right) \\
&\quad - \frac{\partial^2}{\partial x_1^2} y\left(\frac{m_{\eta_1, \ell} + m_{-\eta_1, \ell}}{2}, \frac{m_{\eta_2, \ell} + m_{-\eta_2, \ell}}{2}\right) \left(\frac{x_{\ell_1 + \eta_1 e_1} - x_{\ell_1}}{2}\right) \\
&\quad - \frac{\partial^2}{\partial x_1 \partial x_2} y\left(\frac{m_{\eta_1, \ell} + m_{-\eta_1, \ell}}{2}, \frac{m_{\eta_2, \ell} + m_{-\eta_2, \ell}}{2}\right) \\
&\quad \left(\frac{x_{\ell_2 + \eta_2 e_2} - x_{\ell_2}}{2}\right) + \mathcal{O}\left(\frac{x_{\ell_2 + \eta_2 e_2} - x_{\ell_2}}{2}, \frac{x_{\ell_1 + \eta_1 e_1} - x_{\ell_1}}{2}\right)^2,
\end{aligned} \tag{6.25}$$

then

$$\begin{aligned}
\frac{\partial}{\partial x_1} y(m_{\eta_1, \ell}, m_{\eta_2, \ell}) + \frac{\partial}{\partial x_1} y(m_{-\eta_1, \ell}, m_{-\eta_2, \ell}) &= \frac{\partial}{\partial x_1} y\left(\frac{m_{\eta_1, \ell} + m_{-\eta_1, \ell}}{2}, \frac{m_{\eta_2, \ell} + m_{-\eta_2, \ell}}{2}\right) \\
&\quad + \mathcal{O}(\varepsilon^2),
\end{aligned} \tag{6.26}$$

and similarly,

$$\begin{aligned}
\frac{\partial}{\partial x_2} y(m_{\eta_1, \ell}, m_{\eta_2, \ell}) + \frac{\partial}{\partial x_2} y(m_{-\eta_1, \ell}, m_{-\eta_2, \ell}) &= \frac{\partial}{\partial x_2} y\left(\frac{m_{\eta_1, \ell} + m_{-\eta_1, \ell}}{2}, \frac{m_{\eta_2, \ell} + m_{-\eta_2, \ell}}{2}\right) \\
&\quad + \mathcal{O}(\varepsilon^2).
\end{aligned} \tag{6.27}$$

By substituting (6.24)-(6.27) into (6.23) yields

$$\begin{aligned}
&\frac{\eta_1}{2} \frac{\partial}{\partial x_1} y(m_{\eta_1, \ell}, m_{\eta_2, \ell}) + \frac{\eta_2}{2} \frac{\partial}{\partial x_2} y(m_{\eta_1, \ell}, m_{\eta_2, \ell}) + \frac{\eta_1}{2} \frac{\partial}{\partial x_1} y(m_{-\eta_1, \ell}, m_{-\eta_2, \ell}) \\
&+ \frac{\eta_2}{2} \frac{\partial}{\partial x_2} y(m_{-\eta_1, \ell}, m_{-\eta_2, \ell}) = \eta_1 \frac{\partial}{\partial x_1} y\left(\frac{m_{\eta_1, \ell} + m_{-\eta_1, \ell}}{2}, \frac{m_{\eta_2, \ell} + m_{-\eta_2, \ell}}{2}\right) \\
&\quad + \eta_2 \frac{\partial}{\partial x_2} y\left(\frac{m_{\eta_1, \ell} + m_{-\eta_1, \ell}}{2}, \frac{m_{\eta_2, \ell} + m_{-\eta_2, \ell}}{2}\right) + \mathcal{O}(\varepsilon^2) \\
&= \nabla y(x_{\ell_1}, x_{\ell_2}) \eta + \mathcal{O}(\varepsilon^2).
\end{aligned} \tag{6.28}$$

By following similar steps, we have that

$$\left| \frac{\bar{D}_\eta y_{\ell+e_1+e_2} - \bar{D}_{-\eta} y_{\ell+e_1+e_2}}{2} - \nabla y(x_{\ell+e_1+e_2})\eta \right| \leq \mathcal{O}(\varepsilon^2), \quad (6.29)$$

and similarly,

$$\left| \frac{\bar{D}_{\eta'} y_{\ell+e_1+e_2} - \bar{D}_{-\eta'} y_{\ell+e_1+e_2}}{2} - \nabla y(x_{\ell+e_1+e_2})\eta' \right| \leq \mathcal{O}(\varepsilon^2). \quad (6.30)$$

□

**Lemma 26.** *Under standard smoothness assumptions on  $y$ , an interatomic potential  $\phi$  that is both Lipschitz continuous and satisfies the symmetry property*

$$\phi(\bar{D}_\eta y_\ell, \bar{D}_{\eta'} y_\ell) = \phi(-\bar{D}_{-\eta} y_\ell, -\bar{D}_{-\eta'} y_\ell), \quad (6.31)$$

*we have the following bound*

$$\begin{aligned} & \left| \varepsilon^2 \sum_{\ell \in \mathcal{L}} \sum_{\eta, \eta' \in R} \phi\left(\frac{\bar{D}_\eta y_\ell - \bar{D}_{-\eta} y_\ell}{2}, \frac{\bar{D}_{\eta'} y_\ell - \bar{D}_{-\eta'} y_\ell}{2}\right) \right. \\ & \quad \left. - \varepsilon^2 \sum_{\ell \in \mathcal{L}} \sum_{\eta, \eta' \in R} \phi(\nabla y(x_{\ell_1}, x_{\ell_2})\eta, \nabla y(x_{\ell_1}, x_{\ell_2})\eta') \right| \\ & \leq C \varepsilon^2. \end{aligned} \quad (6.32)$$

*Proof.* By applying the Lipschitz condition

$$|\phi(v_1, v_2) - \phi(\tilde{v}_1, \tilde{v}_2)| \leq c(|v_1 - \tilde{v}_1| + |v_2 - \tilde{v}_2|), \quad (6.33)$$

we obtain

$$\begin{aligned} & \left| \phi\left(\frac{\bar{D}_\eta y_\ell - \bar{D}_{-\eta} y_\ell}{2}, \frac{\bar{D}_{\eta'} y_\ell - \bar{D}_{-\eta'} y_\ell}{2}\right) - \phi(\nabla y(x_{\ell_1}, x_{\ell_2})\eta, \nabla y(x_{\ell_1}, x_{\ell_2})\eta') \right| \\ & \leq c \left( \left| \frac{\bar{D}_\eta y_\ell - \bar{D}_{-\eta} y_\ell}{2} - \nabla y(x_{\ell_1}, x_{\ell_2})\eta \right| + \left| \frac{\bar{D}_{\eta'} y_\ell - \bar{D}_{-\eta'} y_\ell}{2} - \nabla y(x_{\ell_1}, x_{\ell_2})\eta' \right| \right). \end{aligned} \quad (6.34)$$

By implementing Lemma 25 the following holds

$$\left| \phi\left(\frac{\bar{D}_\eta y_\ell - \bar{D}_{-\eta} y_\ell}{2}, \frac{\bar{D}_{\eta'} y_\ell - \bar{D}_{-\eta'} y_\ell}{2}\right) - \phi(\nabla y(x_{\ell_1}, x_{\ell_2})\eta, \nabla y(x_{\ell_1}, x_{\ell_2})\eta') \right| \leq C \varepsilon^2. \quad (6.35)$$

□

Obviously the similar bound holds

$$\begin{aligned} & \left| \varepsilon^2 \sum_{\ell \in \mathcal{L}} \sum_{\eta, \eta' \in R} \phi\left(\frac{\bar{D}_\eta y_{\ell+e_1+e_2} - \bar{D}_{-\eta} y_{\ell+e_1+e_2}}{2}, \frac{\bar{D}_{\eta'} y_{\ell+e_1+e_2} - \bar{D}_{-\eta'} y_{\ell+e_1+e_2}}{2}\right) \right. \\ & \quad \left. - \varepsilon^2 \sum_{\ell \in \mathcal{L}} \sum_{\eta, \eta' \in R} \phi(\nabla y(x_{\ell+e_1+e_2})\eta, \nabla y(x_{\ell+e_1+e_2})\eta') \right| \leq C \varepsilon^2. \end{aligned} \quad (6.36)$$

## 6.3 Main result

The main result of this chapter is the following theorem.

**Theorem 7.** (*Energy Consistency*) Assume  $y$  is a smooth function, and that the interatomic potential  $\phi$  is both Lipschitz continuous and satisfies the symmetry property

$$\phi(\bar{D}_\eta y_\ell, \bar{D}_{\eta'} y_\ell) = \phi(-\bar{D}_{-\eta} y_\ell, -\bar{D}_{-\eta'} y_\ell), \quad (6.37)$$

then the Cauchy-Born continuum energy is a second order approximation to the atomistic energy  $\Phi^a(y)$ : there exists a constant  $M_E = M_E(y)$  such that

$$\left| \Phi^{CB}(y) - \Phi_3^a(y) \right| \leq M_E \varepsilon^2 \quad (6.38)$$

*Proof.* Our starting point is the observation,

$$\begin{aligned} \Phi^{CB}(y) &:= \int_{\Omega} W_{CB}(\nabla y(x)) dx \\ &= \sum_{K \in T} \int_K W_{CB}(\nabla y(x)) dx \\ &= \sum_{K \in T} |K| W_{CB}(\nabla y(m_K)) + \sum_{K \in T} \int_K [W_{CB}(\nabla y(x)) - W_{CB}(\nabla y(m_K))] dx \\ &= I_1 + I_2 \end{aligned} \quad (6.39)$$

where  $m_K$  is the barycenter of cell  $K$  and

$$T := \{K \subset \Omega : K = (x_{\ell_1}, x_{\ell_1+1}) \times (x_{\ell_2}, x_{\ell_2+1}), x_\ell = (x_{\ell_1}, x_{\ell_2}) \in \Omega_{discr}\}. \quad (6.40)$$

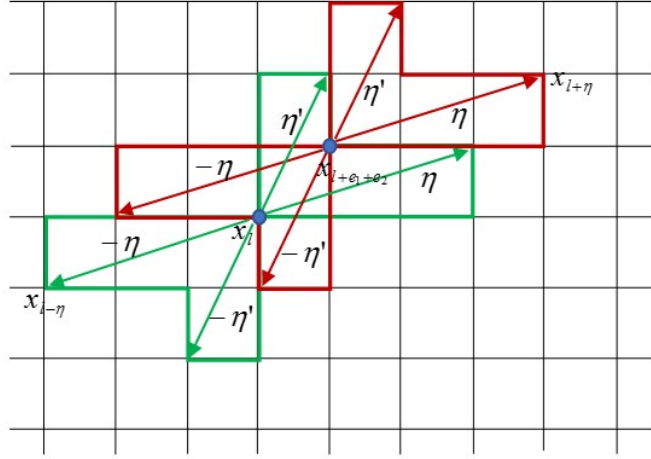
Using similar arguments as in Chapter 4, see also [21], we can verify that  $|I_2| \leq C(y)\varepsilon^2$ . So, it remains for  $I_1$  to be compared with the atomistic energy  $\Phi_3^a(y)$ . The terms in  $\Phi_3^a(y)$  must be rearranged in order to form symmetries around the cell  $K$ . Notice first,

$$\varepsilon^2 \sum_{\ell \in \mathcal{L}} \sum_{\eta, \eta' \in R} \phi(\bar{D}_\eta y_\ell, \bar{D}_{\eta'} y_\ell) = \frac{\varepsilon^2}{2} \sum_{\ell \in \mathcal{L}} \sum_{\eta, \eta' \in R} \phi(\bar{D}_\eta y_\ell, \bar{D}_{\eta'} y_\ell) + \frac{\varepsilon^2}{2} \sum_{\ell \in \mathcal{L}} \sum_{\eta, \eta' \in R} \phi(\bar{D}_\eta y_\ell, \bar{D}_{\eta'} y_\ell). \quad (6.41)$$

For the second term in (6.41), changing the index to  $\ell' = \ell + e_1 + e_2$ , so  $\ell'_1 = \ell_1 + 1$  and  $\ell'_2 = \ell_2 + 1$ , yields,

$$\begin{aligned} \varepsilon^2 \sum_{\ell \in \mathcal{L}} \sum_{\eta, \eta' \in R} \phi(\bar{D}_\eta y_\ell, \bar{D}_{\eta'} y_\ell) &= \frac{\varepsilon^2}{2} \sum_{\ell \in \mathcal{L}} \sum_{\eta, \eta' \in R} \phi(\bar{D}_\eta y_\ell, \bar{D}_{\eta'} y_\ell) \\ &\quad + \frac{\varepsilon^2}{2} \sum_{\ell \in \mathcal{L}} \sum_{\eta, \eta' \in R} \phi(\bar{D}_\eta y_{\ell' + e_1 + e_2}, \bar{D}_{\eta'} y_{\ell' + e_1 + e_2}). \end{aligned} \quad (6.42)$$





**Figure 6.2:** Symmetry due to the combination of  $\bar{D}_{\eta}y_{\ell}$ ,  $\bar{D}_{-\eta}y_{\ell}$ ,  $\bar{D}_{\eta'}y_{\ell}$  and  $\bar{D}_{-\eta'}y_{\ell}$  around the point  $x_{\ell}$  and  $\bar{D}_{\eta}y_{\ell+e_1+e_2}$ ,  $\bar{D}_{-\eta}y_{\ell+e_1+e_2}$ ,  $\bar{D}_{\eta'}y_{\ell+e_1+e_2}$ ,  $\bar{D}_{-\eta'}y_{\ell+e_1+e_2}$  around the point  $x_{\ell+e_1+e_2}$ .

We will drop the apostrophe so that  $\ell' = \ell$  for convenience. Using the symmetry property of the potential (6.37), (6.42) becomes

$$\begin{aligned}
& \frac{\varepsilon^2}{4} \sum_{\ell \in \mathcal{L}} \sum_{\eta, \eta' \in R} \phi(\bar{D}_{\eta}y_{\ell}, \bar{D}_{\eta'}y_{\ell}) + \frac{\varepsilon^2}{4} \sum_{\ell \in \mathcal{L}} \sum_{\eta, \eta' \in R} \phi(-\bar{D}_{-\eta}y_{\ell}, -\bar{D}_{-\eta'}y_{\ell}) \\
& + \frac{\varepsilon^2}{4} \sum_{\ell \in \mathcal{L}} \sum_{\eta, \eta' \in R} \phi(\bar{D}_{\eta}y_{\ell+e_1+e_2}, \bar{D}_{\eta'}y_{\ell+e_1+e_2}) \\
& + \frac{\varepsilon^2}{4} \sum_{\ell \in \mathcal{L}} \sum_{\eta, \eta' \in R} \phi(-\bar{D}_{-\eta}y_{\ell+e_1+e_2}, -\bar{D}_{-\eta'}y_{\ell+e_1+e_2}).
\end{aligned} \tag{6.43}$$

In Figure 6.2,  $\bar{D}_{\eta}y_{\ell}$ ,  $\bar{D}_{-\eta}y_{\ell}$ ,  $\bar{D}_{\eta}y_{\ell+e_1+e_2}$ ,  $\bar{D}_{-\eta}y_{\ell+e_1+e_2}$  and  $\bar{D}_{\eta'}y_{\ell}$ ,  $\bar{D}_{-\eta'}y_{\ell}$ ,  $\bar{D}_{\eta'}y_{\ell+e_1+e_2}$ ,  $\bar{D}_{-\eta'}y_{\ell+e_1+e_2}$  are all displayed. It will be useful to introduce splittings for  $\bar{D}_{\eta}y_{\ell}$ ,  $-\bar{D}_{-\eta}y_{\ell}$ ,  $\bar{D}_{\eta}y_{\ell+e_1+e_2}$ , and  $-\bar{D}_{-\eta}y_{\ell+e_1+e_2}$ :

$$\begin{aligned}
\bar{D}_{\eta}y_{\ell} &= \left\{ \frac{1}{2} \bar{D}_{\eta_1 e_1} y_{\ell} + \frac{1}{2} \bar{D}_{\eta_1 e_1} y_{\ell + \eta_2 e_2} \right\} + \left\{ \frac{1}{2} \bar{D}_{\eta_2 e_2} y_{\ell} + \frac{1}{2} \bar{D}_{\eta_2 e_2} y_{\ell + \eta_1 e_1} \right\} \\
-\bar{D}_{-\eta}y_{\ell} &= \left\{ \frac{1}{2} \bar{D}_{\eta_1 e_1} y_{\ell - \eta} + \frac{1}{2} \bar{D}_{\eta_2 e_2} y_{\ell - \eta_2 e_2} \right\} + \left\{ \frac{1}{2} \bar{D}_{\eta_2 e_2} y_{\ell - \eta} + \frac{1}{2} \bar{D}_{\eta_1 e_1} y_{\ell - \eta_1 e_1} \right\} \\
\bar{D}_{\eta}y_{\ell+e_1+e_2} &= \left\{ \frac{1}{2} \bar{D}_{\eta_1 e_1} y_{\ell+e_1+e_2} + \frac{1}{2} \bar{D}_{\eta_2 e_2} y_{\ell+(\eta_1+1)e_1+e_2} \right\} \\
& + \left\{ \frac{1}{2} \bar{D}_{\eta_2 e_2} y_{\ell+e_1+e_2} + \frac{1}{2} \bar{D}_{\eta_1 e_1} y_{\ell+e_1+(\eta_2+1)e_2} \right\} \\
-\bar{D}_{-\eta}y_{\ell+e_1+e_2} &= \left\{ \frac{1}{2} \bar{D}_{\eta_1 e_1} y_{\ell+(-\eta_1+1)e_1+(-\eta_2+1)e_2} + \frac{1}{2} \bar{D}_{\eta_2 e_2} y_{\ell+e_2+(-\eta_2+1)e_1} \right\} \\
& + \left\{ \frac{1}{2} \bar{D}_{\eta_2 e_2} y_{\ell+(-\eta_1+1)e_1+(-\eta_2+1)e_2} + \frac{1}{2} \bar{D}_{\eta_1 e_1} y_{\ell+(-\eta_1+1)e_1+e_2} \right\},
\end{aligned} \tag{6.44}$$

and similarly for  $\bar{D}_{\eta'}y_{\ell}$ ,  $-\bar{D}_{-\eta'}y_{\ell}$ ,  $\bar{D}_{\eta'}y_{\ell+e_1+e_2}$ , and  $-\bar{D}_{-\eta'}y_{\ell+e_1+e_2}$ . We will now focus on the first two terms of (6.43). By applying Lemmas 24-26 the following holds

$$\begin{aligned}
& \left| \varepsilon^2 \sum_{\ell \in \mathcal{L}} \sum_{\eta, \eta' \in R} \phi(\bar{D}_\eta y_\ell, \bar{D}_{\eta'} y_\ell) - \frac{\varepsilon^2}{2} \sum_{\ell \in \mathcal{L}} \sum_{\eta, \eta' \in R} \phi\left(\nabla y(x_{\ell_1}, x_{\ell_2})\eta, \nabla y(x_{\ell_1}, x_{\ell_2})\eta'\right) \right. \\
& \quad \left. - \frac{\varepsilon^2}{2} \sum_{\ell \in \mathcal{L}} \sum_{\eta, \eta' \in R} \phi\left(\nabla y(x_{\ell_1+1}, x_{\ell_2+1})\eta, \nabla y(x_{\ell_1+1}, x_{\ell_2+1})\eta'\right) \right| \leq C \varepsilon^2.
\end{aligned} \tag{6.45}$$

Therefore, if we set

$$G(x) = \phi(\nabla y(x)\eta, \nabla y(x)\eta'), \tag{6.46}$$

and

$$\bar{x} = (x_{\ell_1}, x_{\ell_2}), \quad \bar{\bar{x}} = (x_{\ell_1+1}, x_{\ell_2+1}), \tag{6.47}$$

to complete the proof of the theorem, it suffices to show that

$$\frac{1}{2}G(\bar{x}) + \frac{1}{2}G(\bar{\bar{x}}) = G(m_K) + \mathcal{O}(\varepsilon^2). \tag{6.48}$$

We apply Taylor expansion to  $G(x_{\ell_1}, x_{\ell_2})$  around  $m_K = (x_{\ell_1+0.5}, x_{\ell_2+0.5})$  which yields

$$\begin{aligned}
G(x_{\ell_1}, x_{\ell_2}) = & G(m_K) - \frac{\partial G}{\partial x}(m_K) \left( \frac{x_{\ell_1+1} - x_{\ell_1}}{2} \right) - \frac{\partial G}{\partial y}(m_K) \left( \frac{x_{\ell_2+1} - x_{\ell_2}}{2} \right) \\
& + \frac{1}{2} \left[ \frac{\partial^2 G}{\partial x^2}(m_K) \left( \frac{x_{\ell_1+1} - x_{\ell_1}}{2} \right)^2 + \frac{\partial^2 G}{\partial y^2}(m_K) \left( \frac{x_{\ell_2+1} - x_{\ell_2}}{2} \right)^2 \right. \\
& \left. + 2 \frac{\partial^2 G}{\partial x \partial y}(m_K) \left( \frac{x_{\ell_1+1} - x_{\ell_1}}{2} \right) \left( \frac{x_{\ell_2+1} - x_{\ell_2}}{2} \right) \right] \\
& + \mathcal{O} \left( \frac{x_{\ell_2+1} - x_{\ell_2}}{2}, \frac{x_{\ell_1+1} - x_{\ell_1}}{2} \right)^3,
\end{aligned} \tag{6.49}$$

and we also apply Taylor expansion to  $G(x_{\ell_1+1}, x_{\ell_2+1})$  around  $m_K$  and we obtain

$$\begin{aligned}
G(x_{\ell_1+1}, x_{\ell_2+1}) = & G(m_K) + \frac{\partial G}{\partial x}(m_K) \left( \frac{x_{\ell_1+1} - x_{\ell_1}}{2} \right) + \frac{\partial G}{\partial y}(m_K) \left( \frac{x_{\ell_2+1} - x_{\ell_2}}{2} \right) \\
& + \frac{1}{2} \left[ \frac{\partial^2 G}{\partial x^2}(m_K) \left( \frac{x_{\ell_1+1} - x_{\ell_1}}{2} \right)^2 + \frac{\partial^2 G}{\partial y^2}(m_K) \left( \frac{x_{\ell_2+1} - x_{\ell_2}}{2} \right)^2 \right. \\
& \left. + 2 \frac{\partial^2 G}{\partial x \partial y}(m_K) \left( \frac{x_{\ell_1+1} - x_{\ell_1}}{2} \right) \left( \frac{x_{\ell_2+1} - x_{\ell_2}}{2} \right) \right] \\
& + \mathcal{O} \left( \frac{x_{\ell_2+1} - x_{\ell_2}}{2}, \frac{x_{\ell_1+1} - x_{\ell_1}}{2} \right)^3.
\end{aligned} \tag{6.50}$$

By adding  $G(x_{\ell_1}, x_{\ell_2})$  and  $G(x_{\ell_1+1}, x_{\ell_2+1})$  the following holds

$$\begin{aligned}
\frac{1}{2}G(x_{\ell_1}, x_{\ell_2}) + \frac{1}{2}G(x_{\ell_1+1}, x_{\ell_2+1}) = & G(m_K) + \frac{1}{2} \left[ \frac{\partial^2 G}{\partial x^2}(m_K) \left( \frac{x_{\ell_1+1} - x_{\ell_2}}{2} \right)^2 \right. \\
& + 2 \frac{\partial^2 G}{\partial x \partial y}(m_K) \left( \frac{x_{\ell_1+1} - x_{\ell_1}}{2} \right) \left( \frac{x_{\ell_2+1} - x_{\ell_2}}{2} \right) \\
& \left. + \frac{\partial^2 G}{\partial y^2}(m_K) \left( \frac{x_{\ell_2+1} - x_{\ell_2}}{2} \right)^2 \right] \\
& + \mathcal{O} \left( \frac{x_{\ell_2+1} - x_{\ell_2}}{2}, \frac{x_{\ell_1+1} - x_{\ell_1}}{2} \right)^3.
\end{aligned} \tag{6.51}$$

The proof is therefore complete.  $\square$

# Chapter 7

## Conclusion and Outlook

### 7.1 Conclusion of thesis

In **Chapter 1** we mainly explained the atomistic Cauchy-Born model and the discontinuous bond volume coupling method. In **Chapter 2** we explained the coupled method described in Section 1.3.1 for the one-dimensional case, and we analysed the energy consistency of the method. We proved two theorems in this chapter. The first theorem, Theorem 1, shows that the coupled energy for  $\eta = 2$  is a second order approximation to the atomistic Cauchy-Born energy, as follows

**Theorem 8.** *For a smooth function  $y$  the energy consistency error is of second order as follows*

$$|\Phi_2^{a,CB}(y) - \mathcal{E}_2^D\{y\}| \leq O(\varepsilon^2).$$

The second theorem, Theorem 2, shows that the coupled energy for  $\eta = 3$  is a second order approximation to the atomistic Cauchy-Born energy.

**Theorem 9.** *For a smooth function  $y$  the energy consistency error is of second order as follows*

$$|\Phi_3^{CB}(y) - \mathcal{E}_3^D\{y\}| \leq O(\varepsilon^2).$$

In **Chapter 3** we performed the error analysis for the first variation of the coupled model in comparison to the first variation of the atomistic Cauchy-Born energy in one dimension for  $\eta = 2$ . We explained that it is important to access the quality of the approximation of the coupled model at the first variation level since the ghost-force phenomenon appears at this level. We proved Theorem 3 that shows that the variational consistency error for the one dimensional coupled method is bounded by  $(\varepsilon^2 + \varepsilon^{2-\frac{1}{p}})$  in the discrete  $W^{-1,p}$  norm, as follows

**Theorem 10.** *Let  $y$  be a smooth function; then, for any  $v \in \mathbb{V}_{\varepsilon,Q}$ , there exist a constant  $M_V = M_V(y, p)$ ,  $1 \leq p \leq \infty$ , independent of  $v$ , such that*

$$\left| \langle D\mathcal{E}_2^D\{y\}, v \rangle - \langle D\Phi^{CB}(y), v \rangle_\varepsilon \right| \leq M_V (\varepsilon^2 + \varepsilon^{2-1/p}) |v|_{W^{1,p}(\Omega)}.$$

Also, we obtained some numerical results for the optimisation of the atomistic model and the optimisation of the discontinuous bond volume based coupling method on one dimension for the Lennard-Jones potential and the Morse potential. We considered four different cases for the external forces and we observed that the coupled method performed well in comparison to the atomistic model.

In **Chapter 4** we described a new two dimensional discontinuous coupled method and we analysed its energy consistency. We proved Theorem 5 that shows that the coupled energy for  $\eta = 2$  is a second order approximation to the atomistic Cauchy-Born energy as follows

**Theorem 11.** (*Energy Consistency*) *Let  $y$  be a smooth function, and  $\mathcal{E}_\eta^D\{y\}$  the coupled energy in (4.19) then there exists a constant  $M_E = M_E(y)$ , such that*

$$|\mathcal{E}_2^D\{y\} - \Phi_2^{CB}(y)| \leq M_E \varepsilon^2.$$

In **Chapter 5** we analysed the variational energy for the two dimensional coupled problem. The analysis in this chapter was what led to the construction of a new discontinuous coupled method. We proved Theorem 6 that shows that the variational consistency error for the two dimensional coupled method is bounded by  $(\varepsilon^2 + \varepsilon^{2-\frac{1}{p}})$  in the discrete  $W^{-1,p}$  norm, as follows

**Theorem 12.** *Let  $y$  be a smooth function; then, for any  $v \in \mathbb{V}_{\varepsilon,Q}$ , the atomistic variation  $\langle D\Phi^{CB}(y), v \rangle$  approximates the variation of the coupled discontinuous method  $\langle D\mathcal{E}_2^D\{y\}, v \rangle$  in the sense that there exist a constant  $M_V = M_V(y, p)$ ,  $1 \leq p \leq \infty$ , independent of  $v$ , such that*

$$\left| \langle D\mathcal{E}_2^D\{y\}, v \rangle - \langle D\Phi^{CB}(y), v \rangle_\varepsilon \right| \leq M_V (\varepsilon^2 + \varepsilon^{2-1/p}) \|v\|_{W^{1,p}(\Omega)}.$$

In **Chapter 6** we extended the energy consistency result of [21] to multi-body potentials, specifically three body potentials. We obtained the first consistency results in the literature for three-body potentials using the atomistic Cauchy-Born models and finite elements. We proved Theorem 7 that shows that the Cauchy-Born continuum energy is a second order approximation to the atomistic energy if we assume that the interatomic potential satisfies the symmetry property, as follows

**Theorem 13.** *Assume  $y$  is a smooth function, and that the interatomic potential  $\phi$  is both Lipschitz continuous and satisfies the symmetry property*

$$\phi(\bar{D}_\eta y_\ell, \bar{D}_{\eta'} y_\ell) = \phi(-\bar{D}_{-\eta} y_\ell, -\bar{D}_{-\eta'} y_\ell),$$

*then the Cauchy-Born continuum energy is a second order approximation to the atomistic energy  $\Phi^a(y)$ : there exists a constant  $M_E = M_E(y)$  such that*

$$\left| \Phi^{CB}(y) - \Phi_3^a(y) \right| \leq M_E \varepsilon^2.$$

## 7.2 Future work

We describe possible future work on atomistic-continuum coupled methods. As a general remark, we note that progress in this field is rather slow due to the very complicated nature of the models involved. Direct extensions of this work will be the study of analytical issues of the methods considered from various perspectives: stability analysis and the effect of penalty stabilisation terms, a posteriori error control and adaptive model selection and full analysis of the nonlinear problem using versions of inverse function theorem. A quite challenging problem is to design discontinuous coupling methods for the three body problem and to achieve a desired order for the energy consistency and variational consistency. The difficulty is in treating the interface terms. Here the three body potential depends on  $\overline{D}_\eta y_\ell$  and  $\overline{D}_{\eta'} y_\ell$  and the first variation cannot be treated by extending the techniques of Chapter 5 in a straightforward way. Another option would be to study time dependent atomistic to continuum couplings. In this thesis we only investigated static methods. The discontinuous interface method could be implemented in combination with Leap-frog and followed by a numerical study of the possible reflections of the boundary. The model could then be modified to yield non-reflecting coupling conditions. It would be interesting to study dynamic methods to see how the system evolves in time. Another option is to develop an atomistic to continuum coupling method for multi-lattice crystals. This is largely an open problem and we hope that the ideas presented herein might be useful in the design of consistent methods in this case.

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# Appendix A

## First Variation of Energy on the Interface used in Chapter 5

The calculations in this appendix are for the purposes of Section 5.2.3. We will compute the first variation of  $E_{2,\Gamma_1}\{y\}$  but only for the  $\overline{D}_{e_2}$  terms since the computations for the  $\overline{D}_{e_1}$  terms are similar. The  $E_{2,\Gamma_1}\{y\}$  is

$$\begin{aligned}
E_{2,\Gamma_1}\{y\} = & -\frac{\varepsilon^2}{4} \sum_{\ell_1=N^*}^{N^{**}-1} \nabla_\zeta \phi(\overline{D}_\eta y(x_{\ell_1}, x_{N^{**}-1})) [\overline{D}_{e_2} y(x_{\ell_1}, x_{N^{**}-1}) - \overline{D}_{e_2} y(x_{\ell_1}, x_{N^{**}})] \\
& -\frac{\varepsilon^2}{4} \sum_{\ell_1=N^*}^{N^{**}-1} \nabla_\zeta \phi(\overline{D}_\eta y(x_{\ell_1-2}, x_{N^{**}-1})) [\overline{D}_{e_2} y(x_{\ell_1}, x_{N^{**}-1}) - \overline{D}_{e_2} y(x_{\ell_1}, x_{N^{**}})] \\
& -\frac{\varepsilon^2}{4} \sum_{\ell_1=N^*}^{N^{**}-1} \nabla_\zeta \phi(\overline{D}_\eta y(x_{\ell_1}, x_{N^{**}-1})) [\overline{D}_{e_1} y(x_{\ell_1}, x_{N^{**}+1}) - \overline{D}_{e_1} y(x_{\ell_1}, x_{N^{**}-1})] \\
& -\frac{\varepsilon^2}{4} \sum_{\ell_1=N^*}^{N^{**}-1} \nabla_\zeta \phi(\overline{D}_\eta y(x_{\ell_1-1}, x_{N^{**}-1})) [\overline{D}_{e_1} y(x_{\ell_1}, x_{N^{**}+1}) \\
& - \overline{D}_{e_1} y(x_{\ell_1}, x_{N^{**}-1})].
\end{aligned} \tag{A.1}$$

The first variation of  $E_{2,\Gamma_1}\{y\}$  in the  $e_2$  direction is computed as follows

$$\begin{aligned}
\langle DE_{2,\Gamma_1}\{y + tv\}, v \rangle_{e_2} = & -\frac{\varepsilon^2}{4} \sum_{\ell_1=N^*}^{N^{**}-1} \frac{d}{dt} \left\{ \frac{\partial \phi}{\partial \zeta_1} \phi(\overline{D}_\eta(y(x_{\ell_1}, x_{N^{**}-1})) + tv(x_{\ell_1}, x_{N^{**}-1})) \right. \\
& [\overline{D}_{e_2}(y(x_{\ell_1}, x_{N^{**}-1}) + tv(x_{\ell_1}, x_{N^{**}-1})) - \overline{D}_{e_2}(y(x_{\ell_1}, x_{N^{**}}) + v(x_{\ell_1}, x_{N^{**}}))]_1 \\
& + \frac{\partial \phi}{\partial \zeta_2} \phi(\overline{D}_\eta(y(x_{\ell_1}, x_{N^{**}-1})) + tv(x_{\ell_1}, x_{N^{**}-1})) [\overline{D}_{e_2}(y(x_{\ell_1}, x_{N^{**}-1}) \\
& + tv(x_{\ell_1}, x_{N^{**}-1})) - \overline{D}_{e_2}(y(x_{\ell_1}, x_{N^{**}}) + v(x_{\ell_1}, x_{N^{**}}))]_2 \Big\} \\
& -\frac{\varepsilon^2}{4} \sum_{\ell_1=N^*}^{N^{**}-1} \frac{d}{dt} \left\{ \frac{\partial \phi}{\partial \zeta_1} \phi(\overline{D}_\eta(y(x_{\ell_1-2}, x_{N^{**}-1})) + tv(x_{\ell_1-2}, x_{N^{**}-1})) [\overline{D}_{e_2}(y(x_{\ell_1}, x_{N^{**}-1}) \right. \\
& + tv(x_{\ell_1}, x_{N^{**}-1})) - \overline{D}_{e_2}(y(x_{\ell_1}, x_{N^{**}}) + v(x_{\ell_1}, x_{N^{**}}))]_1
\end{aligned} \tag{A.2}$$

$$\begin{aligned}
& + \frac{\partial \phi}{\partial \zeta_2} \phi(\overline{D}_\eta(y(x_{\ell_1-2}, x_{N^{**}-1})) + tv(x_{\ell_1-2}, x_{N^{**}-1})) [\overline{D}_{e_2}(y(x_{\ell_1}, x_{N^{**}-1}) \\
& + tv(x_{\ell_1}, x_{N^{**}-1})) - \overline{D}_{e_2}(y(x_{\ell_1}, x_{N^{**}}) + v(x_{\ell_1}, x_{N^{**}}))]_2 \Big\}. \tag{A.3}
\end{aligned}$$

Hence,

$$\begin{aligned}
\langle DE_{\Gamma_1}\{y + tv\}, v \rangle_{e_2} &= -\frac{\varepsilon^2}{4} \sum_{\ell_1=N^*}^{N^{**}-1} \left\{ \frac{\partial^2}{\partial \zeta_1^2} \phi(\overline{D}_\eta(y(x_{\ell_1}, x_{N^{**}-1})) + tv(x_{\ell_1}, x_{N^{**}-1})) \right. \\
& [\overline{D}_{e_2}(y(x_{\ell_1}, x_{N^{**}-1}) + tv(x_{\ell_1}, x_{N^{**}-1})) - \overline{D}_{e_2}(y(x_{\ell_1}, x_{N^{**}}) + tv(x_{\ell_1}, x_{N^{**}}))]_1 \\
& [\overline{D}_\eta(y(x_{\ell_1}, x_{N^{**}-1}))]_1 + \frac{\partial^2}{\partial \zeta_2 \partial \zeta_1} \phi(\overline{D}_\eta(y(x_{\ell_1}, x_{N^{**}-1})) + tv(x_{\ell_1}, x_{N^{**}-1})) \\
& [\overline{D}_{e_2}(y(x_{\ell_1}, x_{N^{**}-1}) + tv(x_{\ell_1}, x_{N^{**}-1})) - \overline{D}_{e_2}(y(x_{\ell_1}, x_{N^{**}}) + tv(x_{\ell_1}, x_{N^{**}}))]_1 \\
& [\overline{D}_\eta(y(x_{\ell_1}, x_{N^{**}-1}))]_2 + \frac{\partial^2}{\partial \zeta_1 \partial \zeta_2} \phi(\overline{D}_\eta(y(x_{\ell_1}, x_{N^{**}-1})) + tv(x_{\ell_1}, x_{N^{**}-1})) \\
& [\overline{D}_{e_2}(y(x_{\ell_1}, x_{N^{**}-1}) + tv(x_{\ell_1}, x_{N^{**}-1})) - \overline{D}_{e_2}(y(x_{\ell_1}, x_{N^{**}}) + tv(x_{\ell_1}, x_{N^{**}}))]_2 \\
& [\overline{D}_\eta(y(x_{\ell_1}, x_{N^{**}-1}))]_1 + \frac{\partial^2}{\partial \zeta_2^2} \phi(\overline{D}_\eta(y(x_{\ell_1}, x_{N^{**}-1})) + tv(x_{\ell_1}, x_{N^{**}-1})) \\
& [\overline{D}_{e_2}(y(x_{\ell_1}, x_{N^{**}-1}) + tv(x_{\ell_1}, x_{N^{**}-1})) - \overline{D}_{e_2}(y(x_{\ell_1}, x_{N^{**}}) + tv(x_{\ell_1}, x_{N^{**}}))]_2 \\
& [\overline{D}_\eta(y(x_{\ell_1}, x_{N^{**}-1}))]_2 \Big\} - \frac{\varepsilon^2}{4} \sum_{\ell_1=N^*}^{N^{**}-1} \left\{ \frac{\partial^2}{\partial \zeta_1^2} \phi(\overline{D}_\eta(y(x_{\ell_1-2}, x_{N^{**}-1})) + tv(x_{\ell_1-2}, x_{N^{**}-1})) \right. \\
& [\overline{D}_{e_2}(y(x_{\ell_1}, x_{N^{**}-1}) + tv(x_{\ell_1}, x_{N^{**}-1})) - \overline{D}_{e_2}(y(x_{\ell_1}, x_{N^{**}}) + tv(x_{\ell_1}, x_{N^{**}}))]_1 \\
& [\overline{D}_\eta(y(x_{\ell_1}, x_{N^{**}-1}))]_1 + \frac{\partial^2}{\partial \zeta_2 \partial \zeta_1} \phi(\overline{D}_\eta(y(x_{\ell_1-2}, x_{N^{**}-1})) + tv(x_{\ell_1-2}, x_{N^{**}-1})) \\
& [\overline{D}_{e_2}(y(x_{\ell_1}, x_{N^{**}-1}) + tv(x_{\ell_1}, x_{N^{**}-1})) - \overline{D}_{e_2}(y(x_{\ell_1}, x_{N^{**}}) + tv(x_{\ell_1}, x_{N^{**}}))]_1 \\
& [\overline{D}_\eta(y(x_{\ell_1}, x_{N^{**}-1}))]_2 + \frac{\partial^2}{\partial \zeta_1 \partial \zeta_2} \phi(\overline{D}_\eta(y(x_{\ell_1-2}, x_{N^{**}-1})) + tv(x_{\ell_1-2}, x_{N^{**}-1})) \\
& [\overline{D}_{e_2}(y(x_{\ell_1}, x_{N^{**}-1}) + tv(x_{\ell_1}, x_{N^{**}-1})) - \overline{D}_{e_2}(y(x_{\ell_1}, x_{N^{**}}) + tv(x_{\ell_1}, x_{N^{**}}))]_2 \\
& [\overline{D}_\eta(y(x_{\ell_1}, x_{N^{**}-1}))]_1 + \frac{\partial^2}{\partial \zeta_2^2} \phi(\overline{D}_\eta(y(x_{\ell_1-2}, x_{N^{**}-1})) + tv(x_{\ell_1-2}, x_{N^{**}-1})) \\
& [\overline{D}_{e_2}(y(x_{\ell_1}, x_{N^{**}-1}) + tv(x_{\ell_1}, x_{N^{**}-1})) - \overline{D}_{e_2}(y(x_{\ell_1}, x_{N^{**}}) + tv(x_{\ell_1}, x_{N^{**}}))]_2 \\
& [\overline{D}_\eta(y(x_{\ell_1}, x_{N^{**}-1}))]_2 \Big\} - \frac{\varepsilon^2}{4} \sum_{\ell_1=N^*}^{N^{**}-1} \left\{ \frac{\partial}{\partial \zeta_1} \phi(\overline{D}_\eta(y(x_{\ell_1}, x_{N^{**}-1})) + tv(x_{\ell_1}, x_{N^{**}-1})) \right. \\
& [\overline{D}_{e_2}(v(x_{\ell_1}, x_{N^{**}-1}) - \overline{D}_{e_2}(y(x_{\ell_1}, x_{N^{**}}))]_1 \\
& + \frac{\partial}{\partial \zeta_2} \phi(\overline{D}_\eta(y(x_{\ell_1}, x_{N^{**}-1})) + tv(x_{\ell_1}, x_{N^{**}-1})) [\overline{D}_{e_2}(v(x_{\ell_1}, x_{N^{**}-1}) \\
& - \overline{D}_{e_2}(y(x_{\ell_1}, x_{N^{**}}))]_2 \Big\} \\
& - \frac{\varepsilon^2}{4} \sum_{\ell_1=N^*}^{N^{**}-1} \left\{ \frac{\partial}{\partial \zeta_1} \phi(\overline{D}_\eta(y(x_{\ell_1-2}, x_{N^{**}-1})) + tv(x_{\ell_1-2}, x_{N^{**}-1})) [\overline{D}_{e_2}(v(x_{\ell_1}, x_{N^{**}-1}) \right.
\end{aligned}$$

$$\begin{aligned}
& -\bar{D}_{e_2}(y(x_{\ell_1}, x_{N^{**}})]_1 + \frac{\partial}{\partial \zeta_2} \phi(\bar{D}_\eta(y(x_{\ell_1-2}, x_{N^{**}-1})) + tv(x_{\ell_1-2}, x_{N^{**}-1})) \\
& [\bar{D}_{e_2}(v(x_{\ell_1}, x_{N^{**}-1}) - \bar{D}_{e_2}(y(x_{\ell_1}, x_{N^{**}})]_2 \Big\}. \tag{A.4}
\end{aligned}$$

Therefore, setting  $t = 0$  yields,

$$\begin{aligned}
\langle DE_{\Gamma_1}\{y + tv\}, v \rangle_{e_2}|_{t=0} = & -\frac{\varepsilon^2}{4} \sum_{\ell_1=N^*}^{N^{**}-1} \left\{ \nabla_\zeta \frac{\partial}{\partial \zeta_1} \phi(\bar{D}_\eta(y(x_{\ell_1}, x_{N^{**}-1}))) \right. \\
& [\bar{D}_{e_2}y(x_{\ell_1}, x_{N^{**}-1}) - \bar{D}_{e_2}y(x_{\ell_1}, x_{N^{**}})]_1 \bar{D}_\eta v(x_{\ell_1}, x_{N^{**}-1}) \\
& + \nabla_\zeta \frac{\partial}{\partial \zeta_2} \phi(\bar{D}_\eta(y(x_{\ell_1}, x_{N^{**}-1}))) [\bar{D}_{e_2}y(x_{\ell_1}, x_{N^{**}-1}) \\
& - \bar{D}_{e_2}y(x_{\ell_1}, x_{N^{**}})]_2 \bar{D}_\eta v(x_{\ell_1}, x_{N^{**}-1}) \Big\} \\
& -\frac{\varepsilon^2}{4} \sum_{\ell_1=N^*}^{N^{**}-1} \left\{ \nabla_\zeta \frac{\partial}{\partial \zeta_1} \phi(\bar{D}_\eta(y(x_{\ell_1-2}, x_{N^{**}-1}))) \right. \\
& [\bar{D}_{e_2}y(x_{\ell_1}, x_{N^{**}-1}) - \bar{D}_{e_2}y(x_{\ell_1}, x_{N^{**}})]_1 \bar{D}_\eta v(x_{\ell_1-2}, x_{N^{**}-1}) \\
& + \nabla_\zeta \frac{\partial}{\partial \zeta_2} \phi(\bar{D}_\eta(y(x_{\ell_1-2}, x_{N^{**}-1}))) [\bar{D}_{e_2}y(x_{\ell_1}, x_{N^{**}-1}) \\
& - \bar{D}_{e_2}y(x_{\ell_1}, x_{N^{**}})]_2 \bar{D}_\eta v(x_{\ell_1-2}, x_{N^{**}-1}) \Big\} \\
& -\frac{\varepsilon^2}{4} \sum_{\ell_1=N^*}^{N^{**}-1} \left\{ \frac{\partial}{\partial \zeta_1} \phi(\bar{D}_\eta y(x_{\ell_1}, x_{N^{**}-1}))) \right. \\
& [\bar{D}_{e_2}v(x_{\ell_1}, x_{N^{**}-1}) - \bar{D}_{e_2}v(x_{\ell_1}, x_{N^{**}})]_1 \\
& + \frac{\partial}{\partial \zeta_2} \phi(\bar{D}_\eta(y(x_{\ell_1}, x_{N^{**}-1}))) \\
& [\bar{D}_{e_2}v(x_{\ell_1}, x_{N^{**}-1}) - \bar{D}_{e_2}v(x_{\ell_1}, x_{N^{**}})]_2 \Big\} \\
& -\frac{\varepsilon^2}{4} \sum_{\ell_1=N^*}^{N^{**}-1} \left\{ \frac{\partial}{\partial \zeta_1} \phi(\bar{D}_\eta(y(x_{\ell_1-2}, x_{N^{**}-1}))) \right. \\
& [\bar{D}_{e_2}v(x_{\ell_1}, x_{N^{**}-1}) - \bar{D}_{e_2}v(x_{\ell_1}, x_{N^{**}})]_1 \\
& + \frac{\partial}{\partial \zeta_2} \phi(\bar{D}_\eta(y(x_{\ell_1-2}, x_{N^{**}-1}))) \\
& [\bar{D}_{e_2}v(x_{\ell_1}, x_{N^{**}-1}) - \bar{D}_{e_2}v(x_{\ell_1}, x_{N^{**}})]_2 \Big\}. \tag{A.5}
\end{aligned}$$

The first variation of  $E_{2,\Gamma_1}\{y\}$  in the  $e_2$  direction is

$$\begin{aligned}
\langle DE_{\Gamma_1}\{y\}, v \rangle_{e_2} = & -\frac{\varepsilon^2}{4} \sum_{\ell_1=N^*}^{N^{**}-1} \nabla_{\zeta}^2 \phi(\overline{D}_{\eta} y(x_{\ell_1}, x_{N^{**}-1})) [\overline{D}_{e_2} y(x_{\ell_1}, x_{N^{**}-1}) \\
& - \overline{D}_{e_2} y(x_{\ell_1}, x_{N^{**}})] \overline{D}_{\eta} v(x_{\ell_1}, x_{N^{**}-1}) \\
& - \frac{\varepsilon^2}{4} \sum_{\ell_1=N^*}^{N^{**}-1} \nabla_{\zeta}^2 \phi(\overline{D}_{\eta} y(x_{\ell_1-2}, x_{N^{**}-1})) [\overline{D}_{e_2} y(x_{\ell_1}, x_{N^{**}-1}) \\
& - \overline{D}_{e_2} y(x_{\ell_1}, x_{N^{**}})] \overline{D}_{\eta} v(x_{\ell_1-2}, x_{N^{**}-1}) \\
& - \frac{\varepsilon^2}{4} \sum_{\ell_1=N^*}^{N^{**}-1} \nabla_{\zeta} \phi(\overline{D}_{\eta} y(x_{\ell_1}, x_{N^{**}-1})) [\overline{D}_{e_2} v(x_{\ell_1}, x_{N^{**}-1}) \\
& - \overline{D}_{e_2} v(x_{\ell_1}, x_{N^{**}})] \\
& - \frac{\varepsilon^2}{4} \sum_{\ell_1=N^*}^{N^{**}-1} \nabla_{\zeta} \phi(\overline{D}_{\eta} y(x_{\ell_1-2}, x_{N^{**}-1})) [\overline{D}_{e_2} v(x_{\ell_1}, x_{N^{**}-1}) \\
& - \overline{D}_{e_2} v(x_{\ell_1}, x_{N^{**}})].
\end{aligned} \tag{A.6}$$